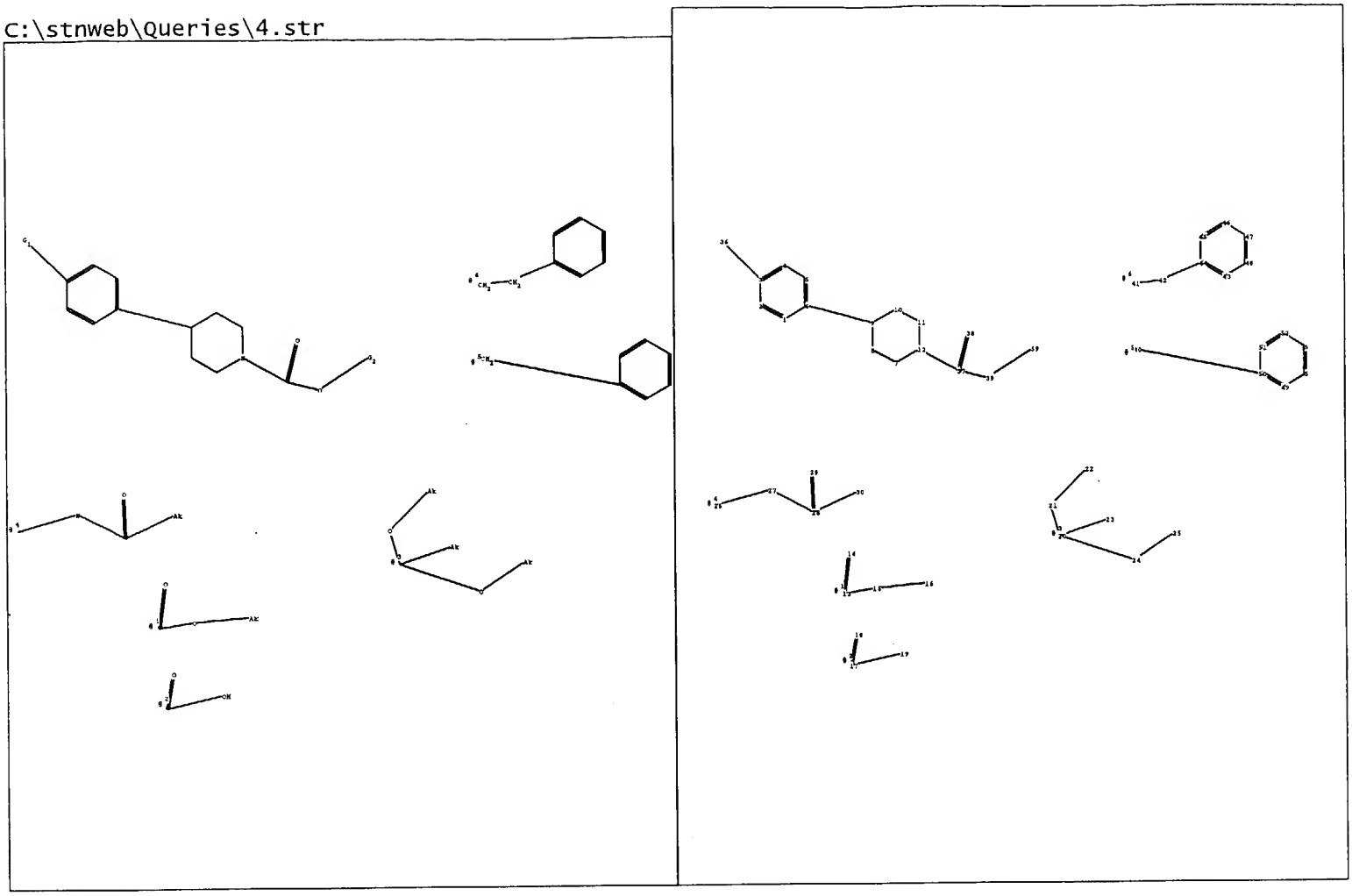
C:\stnweb\Queries\4.str



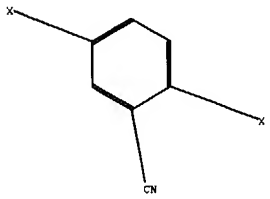
chain nodes :
13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 36 37 38 39
40 41 42 59
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 43 44 45 46 47 48 49 50 51 52 53 54
chain bonds :
3-36 6-9 12-37 13-14 13-15 15-16 17-18 17-19 20-21 20-23 20-24 21-22 24-25
26-27 27-28 28-29 28-30 37-38 37-39 39-59 40-50 41-42 42-44
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 43-44 43-48 44-45
45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53 53-54
exact/norm bonds :
3-36 7-8 7-12 8-9 9-10 10-11 11-12 12-37 13-14 13-15 15-16 20-21 20-23 20-24
21-22 24-25 26-27 27-28 28-29 28-30 37-38 37-39 39-59
exact bonds :
6-9 40-50 41-42 42-44
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-19 43-44 43-48 44-45 45-46 46-47 47-48
49-50 49-54 50-51 51-52 52-53 53-54
isolated ring systems :
containing 1 : 7 : 43 : 49 :

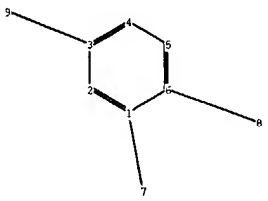
G1:CN,[*1],[*2],[*3],[*4]

G2:Ph,Ak,[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 59:CLASS

C:\stnweb\Queries\6.str

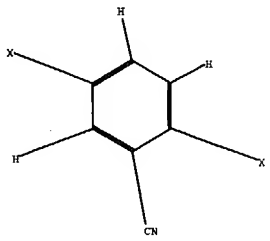


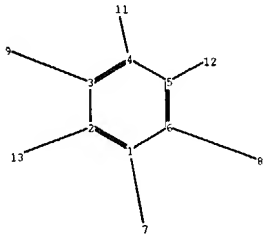


chain nodes :
7 8 9
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 3-9 6-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
1-7 3-9 6-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS

C:\stnweb\Queries\1.str

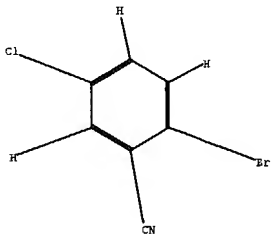


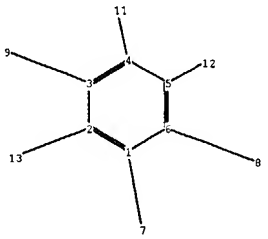


chain nodes :
7 8 9 11 12 13
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 2-13 3-9 4-11 5-12 6-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
1-7 2-13 3-9 4-11 5-12 6-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS

C:\stnweb\Queries\5a.str

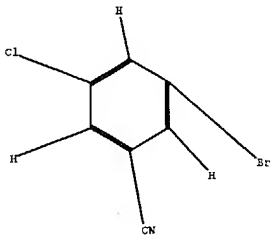


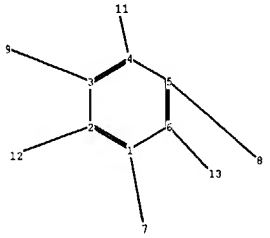


chain nodes :
7 8 9 11 12 13
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 2-13 3-9 4-11 5-12 6-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
1-7 2-13 3-9 4-11 5-12 6-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS

C:\stnweb\Queries\6.str





chain nodes :
7 8 9 11 12 13
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 2-12 3-9 4-11 5-8 6-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
1-7 2-12 3-9 4-11 5-8 6-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS 4	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 5	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 6	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 7	AUG 27	BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 8	AUG 27	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
NEWS 9	SEP 01	INPADOC: New family current-awareness alert (SDI) available
NEWS 10	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS 11	SEP 01	New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 12	SEP 14	STN Patent Forum to be held October 13, 2004, in Iselin, NJ
NEWS 13	SEP 27	STANDARDS will no longer be available on STN
NEWS 14	SEP 27	SWETSCAN will no longer be available on STN
NEWS 15	SEP 30	STN downtime scheduled October 2-3, 2004

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

h eb c g cg b cg eb

DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 14:13:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 37 TO ITERATE

100.0% PROCESSED 37 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 376 TO 1104
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:13:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 821 TO ITERATE

100.0% PROCESSED 821 ITERATIONS 19 ANSWERS
SEARCH TIME: 00.00.01

L3 19 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 160.04 160.25

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
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h eb c g cg b cg eb

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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15
FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l3/thu
            29 L3
        623607 THU/RL
L4           0 L3/THU
                 (L3 (L) THU/RL)

=> d his

     (FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

     FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
L1              STRUCTURE UPLOADED
L2            1 S L1
L3           19 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
L4            0 S L3/THU

=> s l3/prep
            29 L3
       3203746 PREP/RL
L5          27 L3/PREP
                 (L3 (L) PREP/RL)

=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                4.72     164.97

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
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DICTIONARY FILE UPDATES:  29 SEP 2004  HIGHEST RN 754169-63-6

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
```

h eb c g cg b cg eb

http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e pyridinium ion/cn
E1            1     PYRIDINIUM IODINE DIBROMIDE/CN
E2            1     PYRIDINIUM IODINE DICHLORIDE/CN
E3            1 --> PYRIDINIUM ION/CN
E4            1     PYRIDINIUM ION, 3-BROMO-/CN
E5            1     PYRIDINIUM ION, 4-AMINO-/CN
E6            1     PYRIDINIUM ION, 4-BROMO-/CN
E7            1     PYRIDINIUM L-ASCORBATE 2-SULFATE/CN
E8            1     PYRIDINIUM LANOSTEROL SULFATE/CN
E9            1     PYRIDINIUM M-NITROBENZENESULFONATE/CN
E10           1     PYRIDINIUM MER-TRICHLORO(1,2-NAPHTHOQUINONE 1-OXIMATO)(PYRID
                    INE)IRIDATE(1-)/CN
E11           1     PYRIDINIUM MESYLATE/CN
E12           1     PYRIDINIUM METHANESULFONATE/CN

=> s e3
L6            1 "PYRIDINIUM ION"/CN

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     4.85     169.82

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004
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FILE COVERS 1907 - 1 Oct 2004  VOL 141 ISS 15
FILE LAST UPDATED: 30 Sep 2004  (20040930/ED)

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 substance identification.


=> s l6/rct
          717 L6
      2662823 RCT/RL
L7         99 L6/RCT
               (L6 (L) RCT/RL)

=> d his

     (FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

     FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
L1             STRUCTURE UPLOADED
```

h eb c g cg b cg eb

```
L2             1 S L1
L3            19 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
L4             0 S L3/THU
L5            27 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
                E PYRIDINIUM ION/CN
L6             1 S E3

     FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004
L7            99 S L6/RCT

=> s l7 and l5
L8             0 L7 AND L5

=> s l6
L9           717 L6

=> s l9 and l5
L10            0 L9 AND L5

=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY     SESSION
FULL ESTIMATED COST                               2.36      172.18

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004
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STRUCTURE FILE UPDATES:   29 SEP 2004  HIGHEST RN 754169-63-6
DICTIONARY FILE UPDATES:  29 SEP 2004  HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L11      STRUCTURE UPLOADED

=> s l11
SAMPLE SEARCH INITIATED 14:17:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   5872 TO ITERATE

 17.0% PROCESSED    1000 ITERATIONS                          16 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
```

h eb c g cg b cg eb

```
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       112846 TO   122034
PROJECTED ANSWERS:            1298 TO     2460

L12          16 SEA SSS SAM L11

=> s l11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:17:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 116210 TO ITERATE

100.0% PROCESSED  116210 ITERATIONS                          2489 ANSWERS
SEARCH TIME: 00.00.01

L13        2489 SEA SSS FUL L11

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             156.26     328.44

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004
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FILE COVERS 1907 - 1 Oct 2004  VOL 141 ISS 15
FILE LAST UPDATED: 30 Sep 2004  (20040930/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l13
L14          4838 L13

=> s l14 and boice, g?/au
             7 BOICE, G?/AU
L15          1 L14 AND BOICE, G?/AU

=> d l15, ibib abs fhitstr, 1

L15  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2004 ACS on STN
```
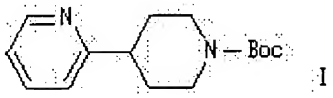

Full Text | Cited References

h eb c g cg b cg eb

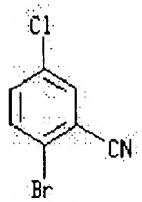
ACCESSION NUMBER: 2004:511300 HCAPLUS
DOCUMENT NUMBER: 141:174054
TITLE: Direct synthesis of 4-arylpiperidines via palladium/copper(I)-cocatalyzed Negishi coupling of a 4-piperidylzinc iodide with aromatic halides and triflates
AUTHOR(S): Corley, Edward G.; Conrad, Karen; Murry, Jerry A.; Savarin, Cecile; Holko, Justin; **Boice, Genevieve**
CORPORATE SOURCE: Departments of Process Research, and Chemical Engineering Research & Development, Merck Research Laboratories, Merck and Co., Inc., Rahway, NJ, 07065, USA
SOURCE: Journal of Organic Chemistry (2004), 69(15), 5120-5123
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB A general procedure for the synthesis of 4-arylpiperidines, e.g., I, via the coupling of 4-(N-Boc-piperidyl)zinc iodide with aryl halides and triflates is presented. The reaction required cocatalysis with both Cl2Pd(dppf) and a copper(I) species. An improved, safer procedure for the activation of zinc dust is also presented.

IT **57381-37-0**, 2-Bromo-5-chlorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-(Boc)-arylpiperidines via addn. of zinc to N-(Boc)-iodopiperidine followed by palladium/copper-catalzyed Negishi coupling with aryl halides and triflates)

RN 57381-37-0 HCAPLUS
CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

h eb c g cg b cg eb

```
L4             0 S L3/THU
L5            27 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
                E PYRIDINIUM ION/CN
L6             1 S E3

     FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004
L7            99 S L6/RCT
L8             0 S L7 AND L5
L9           717 S L6
L10            0 S L9 AND L5

     FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004
L11               STRUCTURE UPLOADED
L12           16 S L11
L13         2489 S L11 FULL

     FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004
L14         4838 S L13
L15            1 S L14 AND BOICE, G?/AU

=> s l14 not l15
L16         4837 L14 NOT L15

=> s l16 and conrad, k?/au
            219 CONRAD, K?/AU
L17           0 L16 AND CONRAD, K?/AU

=> s l16 and corley, e?/au
             59 CORLEY, E?/AU
L18           0 L16 AND CORLEY, E?/AU

=> s l16 and matty, l?/au
             16 MATTY, L?/AU
L19           0 L16 AND MATTY, L?/AU

=> s l16 and murry, j?/au
             60 MURRY, J?/AU
L20           0 L16 AND MURRY, J?/AU

=> s l16 and savarin, c?/au
             14 SAVARIN, C?/AU
L21           0 L16 AND SAVARIN, C?/AU

=> d his

     (FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

     FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
L1                STRUCTURE UPLOADED
L2             1 S L1
L3            19 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
L4             0 S L3/THU
L5            27 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
                E PYRIDINIUM ION/CN
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h eb c g cg b cg eb

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L6            1 S E3

     FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004
L7           99 S L6/RCT
L8            0 S L7 AND L5
L9          717 S L6
L10           0 S L9 AND L5

     FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004
L11             STRUCTURE UPLOADED
L12          16 S L11
L13        2489 S L11 FULL

     FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004
L14        4838 S L13
L15           1 S L14 AND BOICE, G?/AU
L16        4837 S L14 NOT L15
L17           0 S L16 AND CONRAD, K?/AU
L18           0 S L16 AND CORLEY, E?/AU
L19           0 S L16 AND MATTY, L?/AU
L20           0 S L16 AND MURRY, J?/AU
L21           0 S L16 AND SAVARIN, C?/AU

=> d l16, ibib abs fhitstr, 1-10

L16  ANSWER 1 OF 4837  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

ACCESSION NUMBER: 2004:779171 HCAPLUS
TITLE: Indoor air conditioning system containing sustained-release antimicrobial element
INVENTOR(S): Sunagawa, Minoru; Kudo, Toshihiko; Matsuoka, Masayuki
PATENT ASSIGNEE(S): Toshiba Carrier Co., Ltd., Japan; Kodech Chemical K. K.
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

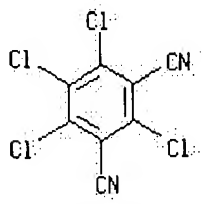
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004263917	A2	20040924	JP 2003-53436	20030228
PRIORITY APPLN. INFO.:			JP 2003-53436	20030228

AB The invention relates to an indoor air conditioning system characterized by including solid antibacterial/antifungal element contg. I2-encapsulated microcapsules and gum rosin, wherein the system shows sustained antimicrobial effect. An indoor air conditioning system having a nonwoven fabric pouch contg. antibacterial/antifungal agent powder with resin and/or wax is also disclosed. A solid antibacterial/antifungal element was prepd. from hydrogenated terpene, dimethylsulfoxide, esterified gum rosin, and I2-encapsulated cyclodextrin for use in an indoor air conditioning system.

IT INDEXING IN PROGRESS
IT **1897-45-6**, 2,4,5,6-Tetrachloroisophthalonitrile
RL: BUU (Biological use, unclassified); DEV (Device component use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(indoor air conditioning system contg. sustained-release antimicrobial element with resin and/or wax)

h eb c g cg b cg eb

RN 1897-45-6 HCAPLUS
CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



L16 ANSWER 2 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:753382 HCAPLUS
TITLE: Preparation of (perfluoroalkyl)benzonitriles
INVENTOR(S): Okumura, Yasunori; Masuda, Takeshi; Nishimae, Shinji; Asako, Yoshinobu
PATENT ASSIGNEE(S): Nippon Shokubai Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

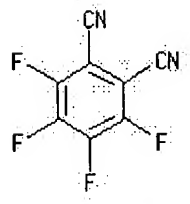
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004256399	A2	20040916	JP 2003-46101	20030224
PRIORITY APPLN. INFO.:			JP 2003-46101	20030224

AB Title compds. I (R1 = perfluoroalkyl; a = 1, 2; b = 1-4; c = 0-4; d = 0-2; a + b + c + d = 6), useful as intermediates for dyes, pharmaceuticals, agrochems., polymers, etc., are prepd. by reaction of tetrafluorophthalonitrile (II) with R2Si(R3)3 (R2 = perfluoroalkyl; R3 = alkyl). II was treated with F3CSiMe3 in N-methylpyrrolidinone-DMF in the presence of CuI and KF at 50° for 8 h to give 9% 3-amino-6-fluoro-4,5-bis(trifluoromethyl)phthalonitrile and 3% 2-amino-5-fluoro-3,4,6-tris(trifluoromethyl)benzonitrile.

IT INDEXING IN PROGRESS

IT **1835-65-0**, Tetrafluorophthalonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of (perfluoroalkyl)benzonitriles from tetrafluorophthalonitrile and perfluoroalkylsilanes)

RN 1835-65-0 HCAPLUS
CN 1,2-Benzenedicarbonitrile, 3,4,5,6-tetrafluoro- (9CI) (CA INDEX NAME)



L16 ANSWER 3 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

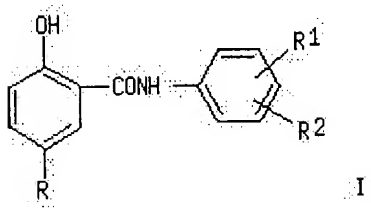
ACCESSION NUMBER: 2004:741848 HCAPLUS
TITLE: Low-pollution antifouling coating compositions

h eb c g cg b cg eb

INVENTOR(S): Kohara, Masanori; Yoshimaru, Masaaki; Morishita, Toshio
PATENT ASSIGNEE(S): Api Corporation, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004250653	A2	20040909	JP 2003-92701	20030221
PRIORITY APPLN. INFO.:			JP 2003-92701	20030221

GI

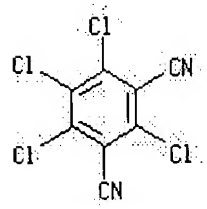


I

AB The coating compns. contain (a) I (R = C1-8 alkyl; R1, R2 = H, C1-4 alkyl, NO2, where R1 and R2 are not H simultaneously) such as 5-tert-butyl-2'-methyl-4'-nitrosalicylanilide, (b) silicone oil, (c) hydrolyzable polymers, and (d) elution control agents such as dialkyl polysulfides and polybutene. The coatings are useful for fish nets, ships, ropes, etc.

IT **1897-45-6**, 1,3-Dicyanotetrachlorobenzene
RL: TEM (Technical or engineered material use); USES (Uses)
(low-pollution antifouling coating compns. contg. salicylanilides)

RN 1897-45-6 HCAPLUS
CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



L16 ANSWER 4 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:740130 HCAPLUS
TITLE: Preparation of pyrazolopurine-based tricyclic compounds for the treatment of inflammatory and immune diseases
INVENTOR(S): Qiu, Yuping; Belema, Makonen; Yang, Xuejie; Zusi, Fred Christopher; Pitts, William J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

h eb c g cg b cg eb

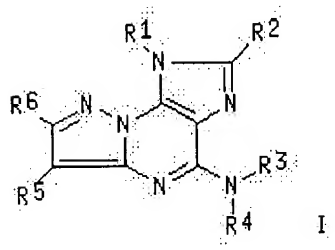
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004075846	A2	20040910	WO 2004-US5384	20040224

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-449770P P 20030225
GI



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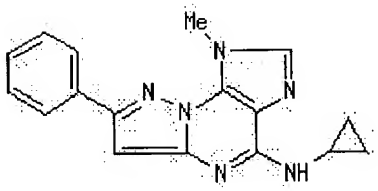


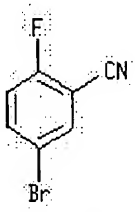
II

AB The title compds. I [R1 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc.; R2 = H, halo, CN, alkyl, alkenyl, alkynyl, etc.; R3 ,R4 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc., or R3R4 together with the nitrogen atom to which they are attached to form a heterocycle; R5 = H, OH, halo, CN, alkyl, alkenyl, alkynyl, etc.] were prepd. for the treatment of inflammatory and immune diseases. For example, reaction of 1-methyl-7-phenyl-4H-pyrazolo[5,1b]purin-4-one (prepn. given) with cyclopropylamine yielded compd. II. The compds. of this invention are active in vitro in the LPS-induced TNFα secretion model.

IT **179897-89-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyrazolopurine-based tricyclic compds. for the treatment of inflammatory and immune diseases)

RN 179897-89-3 HCAPLUS
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



L16 ANSWER 5 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:725629 HCAPLUS
DOCUMENT NUMBER: 141:201726
TITLE: Technology for cultivation of Taishan Polygonum multiflorum
INVENTOR(S): Zhang, Yuqing
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 7 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

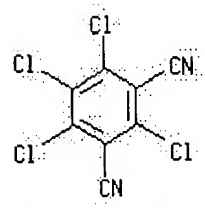
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1408204	A	20030409	CN 2002-130717	20020918
			CN 2002-130717	20020918

PRIORITY APPLN. INFO.:

AB The title technol. comprises the following steps of (1) making pH=6-7 soil into ridge, sterilizing with phoxim and chlorothalonil, flatting soil, watering, sowing 10-15 g/m2 seed, and covering with 2-3 cm thickness soil; (2) spraying seedlings with 1:500 aq. chlorothalonil soln. for 1-3 times, cultivating till the seedlings have 2-4 leaves; (3) harrowing pH=6- 7 soil, applying 3,000-7,000 kg farm manure, ridging, dibbling every 7-10 cm, planting the seedlings, watering, and sealing the holes; setting shelves with height 1.5-2.0 m, and keeping the relative moisture 50-95%.; and (5) picking the seeds, drying, excavating the root tuber at below 10° in the autumn, and packing. The seeds should be sterilized by immersing into aq. carbendazim or chlorothalonil soln. for 20-24 h.

IT **1897-45-6**, Chlorothalonil
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(technol. for cultivation of Taishan Polygonum multiflorum)

RN 1897-45-6 HCAPLUS
CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



L16 ANSWER 6 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:719892 HCAPLUS
DOCUMENT NUMBER: 141:243559
TITLE: Preparation of 3-phenyl-6-(trifluoromethyl)uracils as insecticides

h eb c g cg b cg eb

INVENTOR(S): Schwarz, Hans-Georg; Andree, Roland; Hoischen, Dorothee; Linker, Karl-Heinz; Kluth, Joachim; Schallner, Otto; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf; Loesel, Peter; Auler, Thomas; Hills, Martin; Kehne, Heinz

PATENT ASSIGNEE(S): Bayer CropScience AG, Germany

SOURCE: Ger. Offen., 51 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10307142	A1	20040902	DE 2003-10307142	20030220
WO 2004074274	A1	20040902	WO 2004-EP1198	20040210

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 2003-10307142 A 20030220

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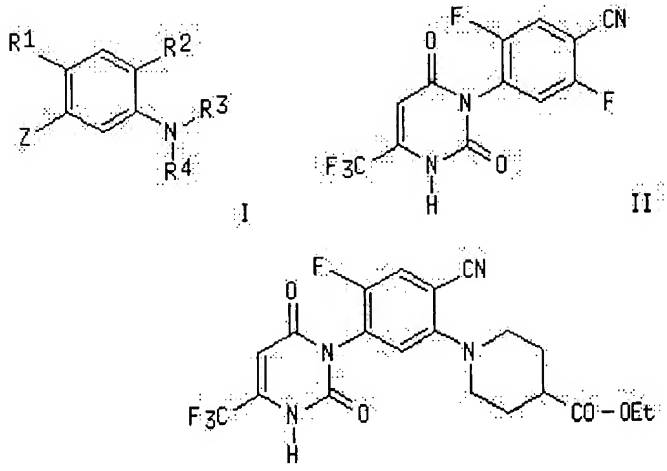


AB Title compds. I [R1 = H, CN, halo; R2 = NO2, CN, thiocarbamoyl; R3, R4 = together with the N-atom form a monocyclic or bicyclic ring with provisos; Z = heterocyclic ring, e.g., s-triazol-3-ols, pyrrole-2,5-diones, 2,4-dioxopyrimidines, etc.] were prepd. For example, N-alkylation of piperidine-4-carboxylic acid Et ester by difluorophenyl II, afforded trifluoromethyluracil III in 40% yield. In spider mite control assays,

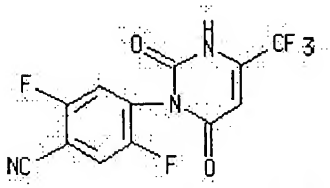
h eb c g cg b cg eb

3-examples of compds. I showed good effectiveness (sic).

IT 162926-25-2, 3-(4-Cyano-2,5-difluorophenyl)-6-trifluoromethyl-1H-pyrimidin-2,4-dione
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of phenyltrifluoromethyluracils as insecticides)

RN 162926-25-2 HCAPLUS

CN Benzonitrile, 4-[3,6-dihydro-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-2,5-difluoro- (9CI) (CA INDEX NAME)



L16 ANSWER 7 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:700578 HCAPLUS
DOCUMENT NUMBER: 141:210090
TITLE: Sulfonated fluorine-containing polyaryl ethers, their compositions, moldings, and polymer electrolyte membranes
INVENTOR(S): Sakaguchi, Yoshimitsu; Kitamura, Kota; Nagahara, Shigenori; Omote, Kazushi; Nishichi, Ai; Asako, Yoshinobu
PATENT ASSIGNEE(S): Toyobo Co., Ltd., Japan; Nippon Shokubai Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004238424	A2	20040826	JP 2003-26294	20030203
PRIORITY APPLN. INFO.:			JP 2003-26294	20030203

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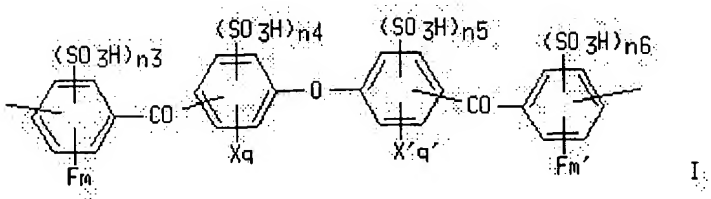

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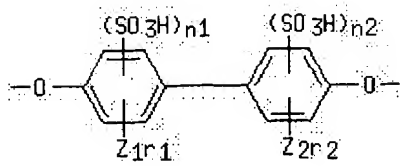


II

AB The polyaryl ethers have repeating units of I [m, m' = 0-4, (m + m') = 1-8; X, X' = halo, C1-6 lower alk(ox)yl; q, q' = 0-4; n1-n6 = 0-2, (n1 + n2 + n3 + n4 + n5 + n6) = 1-12; (n3 + m) ≤4, (n4 + q) ≤4,

h eb c g cg b cg eb

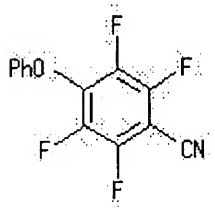
(n5 + q') ≤4, (n6 + m') ≤4] and II [Z1, Z2 = C1-6 lower alkyl, alkoxyl, carboxyl, carbonyl, nitro, amino, OH, halo; r1, r2 = 0-4; (n1 + r1) ≤4, (n2 + r2) ≤4], and/or repeating units of III and IV [s = 1, 2; n7, n8, n9 = 0-2, (n7 + n8 + n9) = 1-6; Z3, Z4 = C1-6 lower alkyl, alkoxyl, carboxyl, carbonyl, nitro, amino, OH, halo; r3, r4 = 0-4; (n7 + r3) ≤4, (n8 + r4) ≤4]. The membranes, useful for fuel cell electrolytes, have desirable amts. of sulfonic acid groups, and show improved ionic cond. and heat resistance.

IT **744229-30-9DP**, sulfonated
RL: DEV (Device component use); IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(sulfonated F-contg. polyaryl ethers for polymer electrolyte membranes with good durability)

RN 744229-30-9 HCAPLUS
CN Benzonitrile, 2,3,5,6-tetrafluoro-4-phenoxy-, polymer with [1,1'-biphenyl]-4,4'-diol and 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (9CI) (CA INDEX NAME)

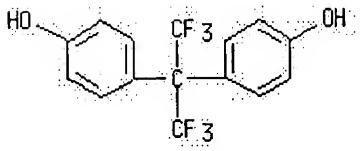
CM 1

CRN 67600-87-7
CMF C13 H5 F4 N O



CM 2

CRN 1478-61-1
CMF C15 H10 F6 O2



CM 3

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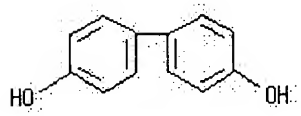

L16 ANSWER 8 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:696342 HCAPLUS

h eb c g cg b cg eb

DOCUMENT NUMBER: 141:225302
TITLE: Preparation of N-arylheterocycles as melanin concentrating hormone (MCH) antagonists.
INVENTOR(S): Schwink, Lothar; Stengelin, Siegfried; Gossel, Matthias; Boehme, Thomas; Hessler, Gerhard; Stahl, Petra; Gretzke, Dirk
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: PCT Int. Appl., 390 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004072025	A2	20040826	WO 2004-EP1342	20040213
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
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DE 10306250	A1	20040909	DE 2003-10306250	20030214
PRIORITY APPLN. INFO.:			DE 2003-10306250	A 20030214

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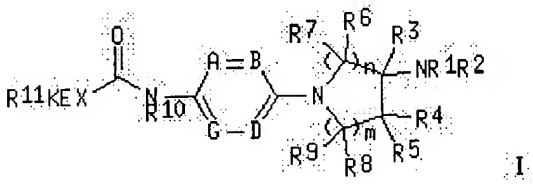


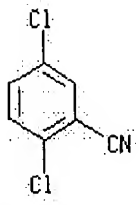
I

AB Title compds. [I; R1, R2 = H, alkyl, alkoxyalkyl, aryloxyalkyl, alkylcarbonyl, alkenylcarbonyl, etc.; R1R2N = atoms to form a 4-10 membered mono-, bi-, or spirocyclic (substituted) ring; R3 = H, alkyl; R4, R5 = H, alkyl, OH, alkoxy, alkylcarbonyloxy, alkylthio; R6-R9 = H, alkyl; R6R7, R8R9 = O; A, B, D, G = N, CR42; AB, DG = CR42; R42 = H, F, Cl, Br, iodo, CF3, NO2, cyano, OCF3, alkoxy, alkylthio, alkenyl, cycloalkyl, cycloalkoxy, cycloalkenyl, alkynyl, CO2H, etc.; R10 = H, alkyl, alkenyl, alkynyl; X = NR52, O, bond, C:C, C≡C, etc.; R52 = H, alkyl; E = (substituted) C3-14 carbocyclyl, heterocyclyl; K = bond, O, CH2O, S, SO, CO, C:C, C≡C, etc.; R11 = H, alkyl, alkoxyalkyl, alkenyl, alkynyl, 3-10 membered (substituted) mono-, bi-, tri- or spirocyclic ring; EKR11 = (unsatd.) tricyclic ring; m, n = 0-2], were prepd. Thus, N-[1-(4-aminophenyl)pyrrolidin-3-yl]piperidine was treated with carbonyldiimidazole and then with 4-(4-chlorophenyl)piperidine to give 4-(4-chlorophenyl)piperidine-1-carboxylic acid [4-[3-(acetylmethylamino)pyrrolidin-1-yl]phenyl]amide. The latter at 30 mg/kg orally in female NMRI mice reduced milk consumption by 64%.

IT **21663-61-6**, 2,5-Dichlorobenzonitrile

h eb c g cg b cg eb

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-arylheterocycles as MCH antagonists)
RN 21663-61-6 HCAPLUS
CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L16 ANSWER 9 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

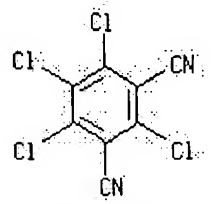
Full Text | Citing References

ACCESSION NUMBER: 2004:683835 HCAPLUS
TITLE: Monitoring of pesticide residues in fresh peaches produced under conventional and integrated crop management cultivation
AUTHOR(S): Tsakiris, I. N.; Danis, T. G.; Stratis, I. A.; Nikitovic, D.; Dialyna, I. A.; Alegakis, A. K.; Tsatsakis, A. M.
CORPORATE SOURCE: Center of Toxicological Sciences and Research, Medical School, University of Crete, Crete, GR-71409, Greece
SOURCE: Food Additives & Contaminants (2004), 21(7), 670-677
CODEN: FACOEB; ISSN: 0265-203X
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The frequency and severity of crop protection product (pesticide) contamination of peaches grown conventionally were compared with those of peaches grown by integrated crop management (ICM). The peach samples (n = 150) were collected preharvest (June-August 2001) from both conventional (n = 55) and ICM (n = 95) cultivations from the Pella and Imathia districts of Macedonia, Northern Greece. The residue levels of selected insecticides, fungicides and acaricides in peach samples were detd. by gas chromatog.-mass spectrometry following solid-phase extn. The concns. of all detected pesticides were lower than the max. residue limits (MRLs) in all peach samples grown with the ICM system ($p < 0.001$). However, chlorpyrifos residues at levels higher than the MRLs were detected in four peach samples (i.e. 7% of the total samples) grown by the conventional system. Comparing the results for both cultivation methods with the reported av. percentage (3.6%) of fruit samples with pesticide residues above the MRLs (European Union report for Greece in 2001), it was concluded that the initial implementation of the ICM in Greece was successful. The present study indicates that ICM cultivation has a higher efficiency in terms of product safety and quality. Furthermore, the results suggest that the application of conventional cultivation requires continuous monitoring of various crop protection product levels.

IT **1897-45-6**, Chlorothalonil
RL: AGR (Agricultural use); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(pesticide residues in fresh peaches produced under conventional and integrated crop management cultivation)
RN 1897-45-6 HCAPLUS
CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

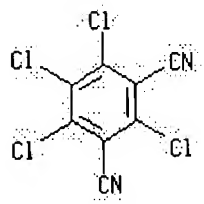
Full Text | Citing References

ACCESSION NUMBER: 2004:682335 HCAPLUS
TITLE: Evaluation of polyaniline as a sorbent for SPE of a variety of polar pesticides from water followed by CD-MEKC-DAD
AUTHOR(S): Bagheri, H.; Saraji, M.; Barcelo, D.
CORPORATE SOURCE: Department of Chemistry, Sharif University of Technology, Tehran, Iran
SOURCE: Chromatographia (2004), 59(5/6), 283-289
CODEN: CHRGB7; ISSN: 0009-5893
PUBLISHER: Vieweg Verlag/GWV Fachverlage GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A recently synthesized polyaniline (PANI) was used and evaluated as a sorbent for solid-phase extn. of a variety of polar pesticides and some of their degrdn. products from H2O samples. Several classes of pesticides including phenoxy acids, triazines, ureas, oxime carbamates and carbamates were selected for this study. The detn. of these pesticides was carried out using cyclodextrin modified micellar electrokinetic chromatog. equipped with diode array detection. The recovery results using PANI were compared with those obtained by C18, Isolute ENV+, Oasis HLB and LiChrolut EN. Effect of humic acid, as a major interference, on extn. recovery was also studied. The performance of the method was evaluated by anal. of tap and river water. The relative std. deviation of method was 6-14% (n = 3) and detection limits were at 0.01-0.5 μg L-1 using 350-mL H2O samples.

IT **1897-45-6**, Chlorothalonil
RL: ANT (Analyte); ANST (Analytical study)
(evaluation of polyaniline as a sorbent for SPE of a variety of polar pesticides from water followed by CD-MEKC-DAD)

RN 1897-45-6 HCAPLUS
CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3             19 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
L4              0 S L3/THU
L5             27 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
                E PYRIDINIUM ION/CN
L6              1 S E3

     FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004
L7             99 S L6/RCT
L8              0 S L7 AND L5
L9            717 S L6
L10             0 S L9 AND L5

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L12            16 S L11
L13          2489 S L11 FULL

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L14          4838 S L13
L15             1 S L14 AND BOICE, G?/AU
L16          4837 S L14 NOT L15
L17             0 S L16 AND CONRAD, K?/AU
L18             0 S L16 AND CORLEY, E?/AU
L19             0 S L16 AND MATTY, L?/AU
L20             0 S L16 AND MURRY, J?/AU
L21             0 S L16 AND SAVARIN, C?/AU

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                59.44     387.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                -7.70      -7.70

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provided by InfoChem.

STRUCTURE FILE UPDATES:   29 SEP 2004  HIGHEST RN 754169-63-6
DICTIONARY FILE UPDATES:  29 SEP 2004  HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L22 HAS NO ANSWERS
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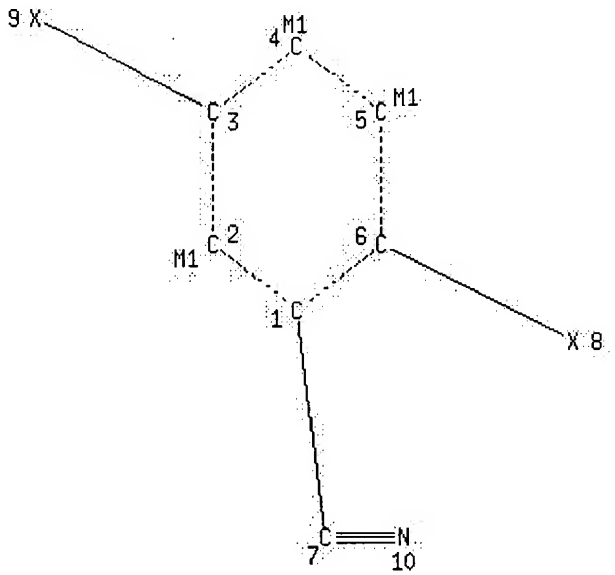

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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

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SAMPLE SCREEN SEARCH COMPLETED - 5872 TO ITERATE

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 17.0% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       112846 TO   122034
PROJECTED ANSWERS:               0 TO        0

L23           0 SEA SSS SAM L22

=> s 122 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:20:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 116210 TO ITERATE

100.0% PROCESSED  116210 ITERATIONS                              24 ANSWERS
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FULL ESTIMATED COST                                   155.84     543.72

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                     0.00      -7.70

FILE 'HCAPLUS' ENTERED AT 14:20:39 ON 01 OCT 2004
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FILE COVERS 1907 - 1 Oct 2004  VOL 141 ISS 15
FILE LAST UPDATED: 30 Sep 2004  (20040930/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L25         206 L24

=> d 125, ibib abs fhitstr, 1-10

L25  ANSWER 1 OF 206  HCAPLUS  COPYRIGHT 2004 ACS on STN
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h eb c g cg b cg eb

Full Text | Citing References

ACCESSION NUMBER: 2004:740130 HCAPLUS
TITLE: Preparation of pyrazolopurine-based tricyclic compounds for the treatment of inflammatory and immune diseases
INVENTOR(S): Qiu, Yuping; Belema, Makonen; Yang, Xuejie; Zusi, Fred Christopher; Pitts, William J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004075846	A2	20040910	WO 2004-US5384	20040224

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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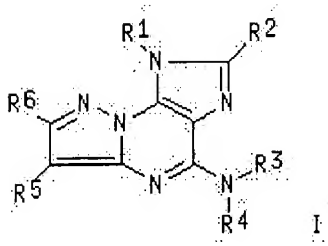

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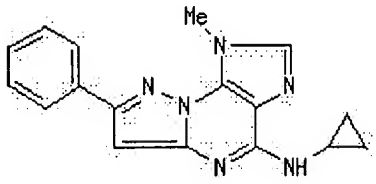


II

AB The title compds. I [R1 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc.; R2 = H, halo, CN, alkyl, alkenyl, alkynyl, etc.; R3 ,R4 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc., or R3R4 together with the nitrogen atom to which they are attached to form a heterocycle; R5 = H, OH, halo, CN, alkyl, alkenyl, alkynyl, etc.] were prepd. for the treatment of inflammatory and immune diseases. For example, reaction of 1-methyl-7-phenyl-4H-

h eb c g cg b cg eb

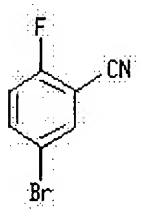
pyrazolo[5,1b]purin-4-one (prepn. given) with cyclopropylamine yielded compd. II. The compds. of this invention are active in vitro in the LPS-induced TNFα secretion model.

IT **179897-89-3**

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyrazolopurine-based tricyclic compds. for the treatment of inflammatory and immune diseases)

RN 179897-89-3 HCAPLUS

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 2 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:696342 HCAPLUS
DOCUMENT NUMBER: 141:225302
TITLE: Preparation of N-arylheterocycles as melanin concentrating hormone (MCH) antagonists.
INVENTOR(S): Schwink, Lothar; Stengelin, Siegfried; Gossel, Matthias; Boehme, Thomas; Hessler, Gerhard; Stahl, Petra; Gretzke, Dirk
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: PCT Int. Appl., 390 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004072025	A2	20040826	WO 2004-EP1342	20040213
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PRIORITY APPLN. INFO.: DE 2003-10306250 A 20030214

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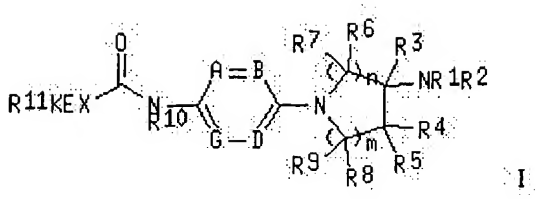


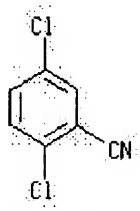
I

AB Title compds. [I; R1, R2 = H, alkyl, alkoxyalkyl, aryloxyalkyl, alkylcarbonyl, alkenylcarbonyl, etc.; R1R2N = atoms to form a 4-10 membered mono-, bi-, or spirocyclic (substituted) ring; R3 = H, alkyl; R4, R5 = H, alkyl, OH, alkoxy, alkylcarbonyloxy, alkylthio; R6-R9 = H, alkyl; R6R7, R8R9 = O; A, B, D, G = N, CR42; AB, DG = CR42; R42 = H, F, Cl, Br, iodo, CF3, NO2, cyano, OCF3, alkoxy, alkylthio, alkenyl, cycloalkyl, cycloalkoxy, cycloalkenyl, alkynyl, CO2H, etc.; R10 = H, alkyl, alkenyl, alkynyl; X = NR52, O, bond, C:C, C≡C, etc.; R52 = H, alkyl; E = (substituted) C3-14 carbocyclyl, heterocyclyl; K = bond, O, CH2O, S, SO, CO, C:C, C≡C, etc.; R11 = H, alkyl, alkoxyalkyl, alkenyl, alkynyl, 3-10 membered (substituted) mono-, bi-, tri- or spirocyclic ring; EKR11 = (unsatd.) tricyclic ring; m, n = 0-2], were prepd. Thus, N-[1-(4-aminophenyl)pyrrolidin-3-yl]piperidine was treated with carbonyldiimidazole and then with 4-(4-chlorophenyl)piperidine to give 4-(4-chlorophenyl)piperidine-1-carboxylic acid [4-[3-(acetylmethylamino)pyrrolidin-1-yl]phenyl]amide. The latter at 30 mg/kg orally in female NMRI mice reduced milk consumption by 64%.

IT **21663-61-6**, 2,5-Dichlorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-arylheterocycles as MCH antagonists)

RN 21663-61-6 HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L25 ANSWER 3 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:675728 HCAPLUS
DOCUMENT NUMBER: 141:207205
TITLE: Preparation of acrylamide derivatives as CCR antagonists
INVENTOR(S): Shiraishi, Mitsuru; Seto, Masaki; Aikawa, Katsuji; Kanzaki, Naoyuki; Baba, Masanori
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 284 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069808	A1	20040819	WO 2004-JP1181	20040205

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,
MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG

JP 2004256530 A2 20040916 JP 2004-29681 20040205
PRIORITY APPLN. INFO.: JP 2003-31068 A 20030207
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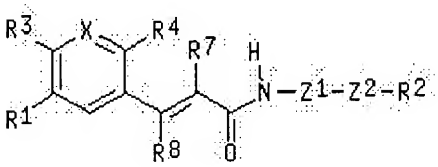

I

AB The title compds. I [R1 represents a 5- or 6-membered ring; R3 represents hydrogen, lower alkyl, or lower alkoxy; R7 and R8 each represents hydrogen or lower alkyl; Z1 represents a 5- or 6-membered arom. ring; Z2 represents a group represented by Z2a-W1-Z2b- (Z2a and Z2b each represents oxygen, S(O)m (m is 0, 1, or 2), imino, or a bond and W1 represents an alkylene chain); X represents CR (R represents hydrogen, lower alkyl, lower alkoxy, or acyl, provided that R may form a 5- or 6-membered alicyclic heterocyclic group in cooperation with the adjacent R4) or nitrogen; R4 represents NR5R6 (R5 and R6 each represents hydrogen, a hydrocarbon group, a heterocyclic group, or acyl, or R5 is bonded to R6 to form a heterocyclic group represented by NR5R6); and R2 represents (1) amino in which the nitrogen atom may be in the form of a quaternary ammonium or oxide, (2) a nitrogenous heterocyclic group in which the ring-constituting atoms may include a sulfur or oxygen atom and the nitrogen atom may be in the form of a quaternary ammonium or oxide, etc.] are prepd. For example, (S)-(2E)-3-[4-Azepan-1-yl-4'-(2-butoxyethoxy)-1,1'-biphenyl-3-yl]-N-[4-[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]phenyl]acrylamide was prepd. from (2E)-3-[4-azepan-1-yl-4'-(2-butoxyethoxy)-1,1'-biphenyl-3-yl]acrylic acid and (S)-4-[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]aniline. I have excellent antagonistic activity against CCR5 and are useful as preventive/therapeutic agents for diseases caused by HIV infection in human peripheral blood mononuclear cells, esp. for AIDS. In an in vitro assay for CCR5 antagonism, compds. of this invention at 1 μM gave 89% to 100% CCR5 binding inhibition. Formulations are given.

IT **179897-89-3**, 5-Bromo-2-fluorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of acrylamide derivs. as CCR antagonists)

RN 179897-89-3 HCAPLUS
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)

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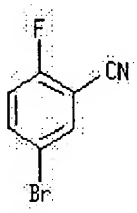

L25 ANSWER 4 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:648523 HCAPLUS
DOCUMENT NUMBER: 141:190682
TITLE: Preparation of indole-derived modulators of steroid hormone nuclear receptors
INVENTOR(S): Bell, Michael Gregory; Gavardinas, Konstantinos; Gernert, Douglas Linn; Grese, Timothy Alan; Jadhav, Prabhakar Kondaji; Lander, Peter Ambrose; Steinberg, Mitchell Irvin
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 243 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067529	A1	20040812	WO 2004-US17	20040120

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI

PRIORITY APPLN. INFO.: US 2003-441947P P 20030122
GI

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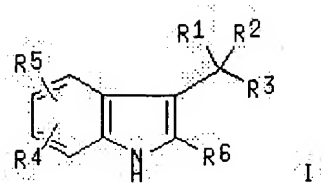

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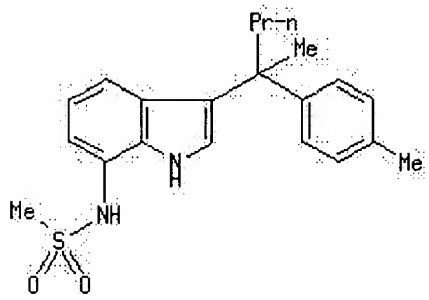


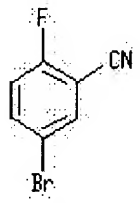
II

AB Title compds. I [R1 = cycloalkyl, alkynyl, aryl, etc.; R2 = alkyl, cycloalkyl, aryl, etc.; R3 = alkyl, haloalkyl, cycloalkyl, etc.; R4 = H, halo, OH, amino, etc.; R5 = H, halo, OH, amino, etc.; R6 = H, halo, alkyl, etc.] are prepd. For instance, N-(1H-indol-7-yl)methanesulfonamide is reacted with the appropriate carbinol (CH2Cl2, TFA) to give II. II has Ki < 500 nM for the mineralocorticorticoid and glucocorticoid receptor. I are useful for treating, e.g., congestive heart disease.

IT **179897-89-3**, 5-Bromo-2-fluorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(indole-deriv. modulators of steroid hormone nuclear receptors)

RN 179897-89-3 HCAPLUS

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 5 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	2004:550742 HCAPLUS
DOCUMENT NUMBER:	141:106471
TITLE:	Preparation of imidazo[4,5-c]pyridin-4-ones as GABAa receptor ligands for the treatment of anxiety, convulsions and cognitive disorders.
INVENTOR(S):	Goodacre, Simon Charles
PATENT ASSIGNEE(S):	UK
SOURCE:	U.S. Pat. Appl. Publ., 14 pp. CODEN: USXXCO
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

h eb c g cg b cg eb

US 2004132767	A1	20040708	US 2003-697210	20031030
PRIORITY APPLN. INFO.:			GB 2002-25399 A	20021031
OTHER SOURCE(S):	MARPAT 141:106471			

GI

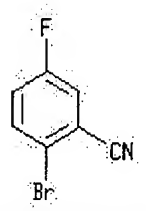
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [X1 = H, halo, alkyl, etc.; X2 = H, halo; Y = bond, O, NH; Z = (un)substituted aryl, heteroaryl; R1 = hydrocarbon, heterocyclic, CF3C, etc.] and their pharmaceutically acceptable salts were prepd. For example, coupling of 3-fluoro-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)pyridine and bromophenyl II e.g., prepd. from 5-fluoropyridin-3-ol in 4-steps, afforded imidazopyridinone III. In human GABAa receptor binding assays, 6-examples of compds. I exhibited Ki values for displacement of [3H]-flumazenil from the α2 and/or α3 and/or α5 subunit of the GABAa receptor of 100 nM or less. Compds. I were claimed useful for the treatment of anxiety, convulsions and cognitive disorders.

IT **57381-39-2**, 2-Bromo-5-fluorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of imidazo[4,5-c]pyridin-4-ones as GABAa receptor ligands for the treatment of anxiety, convulsions and cognitive disorders.)

RN 57381-39-2 HCAPLUS

CN Benzonitrile, 2-bromo-5-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 6 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	2004:523233 HCAPLUS
DOCUMENT NUMBER:	141:207126
TITLE:	Pd-Cu catalyzed heterocyclization during Sonogashira coupling: synthesis of 3-benzylthiazolo[3,2-a]benzimidazole
AUTHOR(S):	Heravi, Majid M.; Keivanloo, Ali; Rahimizadeh, Mohammad; Bakavoli, Mehdi; Ghassemzadeh, Mitra
CORPORATE SOURCE:	Department of Chemistry, School of Sciences, Azzahra University, Tehran, Iran
SOURCE:	Tetrahedron Letters (2004), 45(29), 5747-5749 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:	Elsevier
DOCUMENT TYPE:	Journal
LANGUAGE:	English

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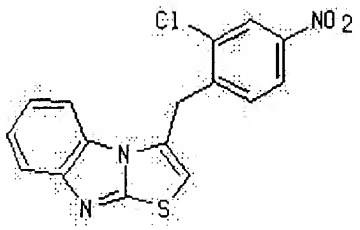
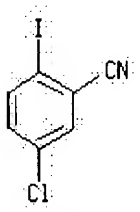


I

AB The reaction of 2-mercaptopropargyl benzimidazole with various iodobenzenes catalyzed by Pd-Cu leads to the formation of 3-benzylthiazolo[3,2-a]benzimidazoles, e.g., I.

IT **549547-88-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzylthiazolobenzimidazoles via palladium-copper catalyzed Sonogashira coupling of mercaptopropargyl benzimidazole with iodobenzenes followed by heterocyclization)

RN 549547-88-8 HCAPLUS
CN Benzonitrile, 5-chloro-2-iodo- (9CI) (CA INDEX NAME)

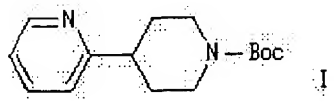


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:511300 HCAPLUS
DOCUMENT NUMBER: 141:174054
TITLE: Direct synthesis of 4-arylpiperidines via palladium/copper(I)-cocatalyzed Negishi coupling of a 4-piperidylzinc iodide with aromatic halides and triflates
AUTHOR(S): Corley, Edward G.; Conrad, Karen; Murry, Jerry A.; Savarin, Cecile; Holko, Justin; Boice, Genevieve
CORPORATE SOURCE: Departments of Process Research, and Chemical Engineering Research & Development, Merck Research Laboratories, Merck and Co., Inc., Rahway, NJ, 07065, USA
SOURCE: Journal of Organic Chemistry (2004), 69(15), 5120-5123
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A general procedure for the synthesis of 4-arylpiperidines, e.g., I, via the coupling of 4-(N-Boc-piperidyl)zinc iodide with aryl halides and

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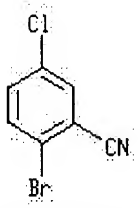
triflates is presented. The reaction required cocatalysis with both Cl2Pd(dppf) and a copper(I) species. An improved, safer procedure for the activation of zinc dust is also presented.

IT **57381-37-0**, 2-Bromo-5-chlorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-(Boc)-arylpiperidines via addn. of zinc to N-(Boc)-iodopiperidine followed by palladium/copper-catalzyed Negishi coupling with aryl halides and triflates)

RN 57381-37-0 HCAPLUS
CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



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L25 ANSWER 8 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2004:412927 HCAPLUS
DOCUMENT NUMBER: 140:423666
TITLE: A preparation of antiinflammatory 3-arylthio-3-thiazolyl-alkylamine derivatives
INVENTOR(S): Stonehouse, Jeffrey
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041794	A1	20040521	WO 2003-SE1712	20031106

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: SE 2002-3304 A 20021107
OTHER SOURCE(S): MARPAT 140:423666
GI

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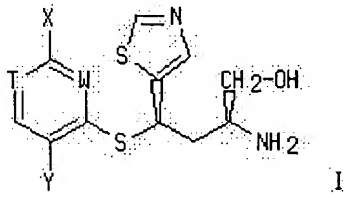

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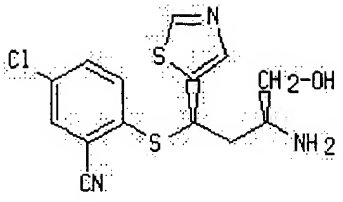

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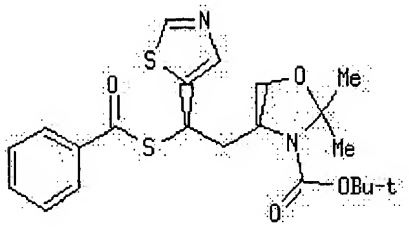
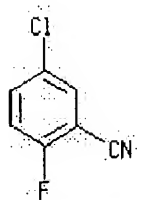


III

AB The invention relates to 3-arylthio-3-thiazolyl-alkylamine derivs. of formula I [wherein: T and W independently represent CR1 or N, when more than one R1 group is present, each may be selected independently; X and R1 independently represent H, C1-4alkyl, halogen, CN, or C≡CH, etc.; Y is C1-4alkyl, C1-4alkoxy, halogen, CN, NO2, or CHO, etc.], useful as antiinflammatory agents. The compds. are inhibitors of nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease and pain. For instance, arylthio(thiazolyl)alkylamine deriv. II (nitric oxide synthase inhibition IC50 < 100 μM) was prepd. via reaction of thiazole deriv. III with 5-chloro-2-fluorobenzonitrile, and subsequent hydrolysis of the obtained product (example 5, no yield data).

IT **57381-34-7**, 5-Chloro-2-fluorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of antiinflammatory arylthio(thiazolyl)alkylamine derivs.)

RN 57381-34-7 HCAPLUS
CN Benzonitrile, 5-chloro-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 9 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:377142 HCAPLUS
DOCUMENT NUMBER: 141:123579
TITLE: Discovery and Evaluation of Potent P1 Aryl Heterocycle-Based Thrombin Inhibitors
AUTHOR(S): Young, Mary Beth; Barrow, James C.; Glass, Kristen L.; Lundell, George F.; Newton, Christina L.; Pellicore, Janetta M.; Rittle, Kenneth E.; Selnick, Harold G.; Stauffer, Kenneth J.; Vacca, Joseph P.; Williams, Peter D.; Bohn, Dennis; Clayton, Franklin C.; Cook, Jacquelynn J.; Krueger, Julie A.; Kuo, Lawrence C.; Lewis, S. Dale; Lucas, Bobby J.; McMasters, Daniel R.;

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Miller-Stein, Cynthia; Pietrak, Beth L.; Wallace, Audrey A.; White, Rebecca B.; Wong, Bradley; Yan, Youwei; Nantermet, Philippe G.

CORPORATE SOURCE: Medicinal Chemistry, Pharmacology, Biological Chemistry, Structural Biology, Molecular Systems and Drug Metabolism, Merck Research Laboratories, Merck and Co. Inc., West Point, PA, 19486, USA

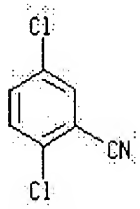
SOURCE: Journal of Medicinal Chemistry (2004), 47(12), 2995-3008
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In an effort to discover potent, clin. useful thrombin inhibitors, a rapid analog synthetic approach was used to explore the P1 region. Various benzylamines were coupled to a pyridine/pyrazinone P2-P3 template. One compd., i.e. 2-[6-chloro-3-(2,2-difluoro-2-pyridin-2-yl-ethylamino)-2-oxo-2H-pyrazin-1-yl]-N-(2-[1,2,3]thiadiazol-4-yl-benzyl)acetamide, was found to have a thrombin Ki of 0.84 nM. A study of ortho-substituted five-membered-ring heterocycles was undertaken and subsequently demonstrated that the o-triazole and tetrazole rings were optimal. Combination of these potent P1 aryl heterocycles with a variety of P2-P3 groups produced a compd. with an extraordinary thrombin inhibitory activity of 1.4 pM. It is hoped that this potency enhancement in P1 will allow for more diversification in the P2-P3 region to ultimately address addnl. pharmacol. concerns.

IT **21663-61-6**, 2,5-Dichlorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of P1 aryl heterocycle-based thrombin inhibitors)

RN 21663-61-6 HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 10 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:365206 HCAPLUS
DOCUMENT NUMBER: 141:88996

TITLE: A single step synthesis of 6-aminophenanthridines from anilines and 2-chlorobenzonitriles

AUTHOR(S): Gug, Fabienne; Bach, Stephane; Blondel, Marc; Vierfond, Jean-Michel; Martin, Anne-Sophie; Galons, Herve

CORPORATE SOURCE: Laboratoire de Chimie Organique, Universite Rene Descartes, Paris, 75006, Fr.

SOURCE: Tetrahedron (2004), 60(21), 4705-4708
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

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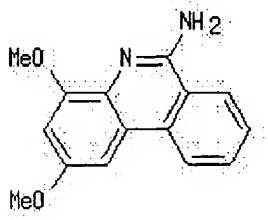


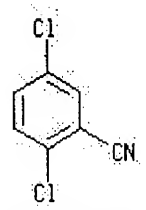
I

AB Biol. active 6-aminophenanthridines, e.g., I, were prepd. in a single step procedure. Metal amides, in liq. ammonia, promoted the condensation of anilines with 2-chloro-benzonitriles. 6-Aminophenanthridines were isolated in moderate yield.

IT **21663-61-6**, 2,5-Dichlorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aminophenanthridines via heterocyclization of anilines with chlorobenzonitriles)

RN 21663-61-6 HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Sep 2004 (20040930/PD)
FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)
HIGHEST GRANTED PATENT NUMBER: US6799328
HIGHEST APPLICATION PUBLICATION NUMBER: US2004194186
CA INDEXING IS CURRENT THROUGH 30 Sep 2004 (20040930/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Sep 2004 (20040930/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2004

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>>> applications. USPAT2 contains full text of the latest US <<<
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>>>  published document but also a list of any subsequent              <<<
>>>  publications.  The publication number, patent kind code, and      <<<
>>>  publication date for all the US publications for an invention     <<<
>>>  are displayed in the PI (Patent Information) field of USPATFULL   <<<
>>>  records and may be searched in standard search fields, e.g., /PN, <<<
>>>  /PK, etc.                                                         <<<

>>>  USPATFULL and USPAT2 can be accessed and searched together        <<<
>>>  through the new cluster USPATALL.  Type FILE USPATALL to          <<<
>>>  enter this cluster.                                               <<<
>>>                                                                    <<<
>>>  Use USPATALL when searching terms such as patent assignees,       <<<
>>>  classifications, or claims, that may potentially change from      <<<
>>>  the earliest to the latest publication.                           <<<

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d his

     (FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

     FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
L1             STRUCTURE UPLOADED
L2               1 S L1
L3              19 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
L4               0 S L3/THU
L5              27 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
                E PYRIDINIUM ION/CN
L6               1 S E3

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L8               0 S L7 AND L5
L9             717 S L6
L10              0 S L9 AND L5

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L11            STRUCTURE UPLOADED
L12             16 S L11
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L22            STRUCTURE UPLOADED
L23              0 S L22
L24             24 S L22 FULL
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h eb c g cg b cg eb

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L25         206 S L24

     FILE 'USPATFULL' ENTERED AT 14:21:07 ON 01 OCT 2004

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L26          99 L24

=> s l26 and pd < april 2003
       3433506 PD < APRIL 2003
                 (PD<20030400)
L27          63 L26 AND PD < APRIL 2003

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L27  ANSWER 1 OF 63  USPATFULL on STN
```

Full Text | Citing References

```
ACCESSION NUMBER:          2004:46802  USPATFULL
TITLE:                     Treatment of asthma with MEK inhibitors
INVENTOR(S):               Bridges, Alexander James, Saline, MI, United States
                           Dudley, David Thomas, Ann Arbor, MI, United States
                           Mobley, James Leslie, Brighton, MI, United States
                           Saltiel, Alan Robert, Ann Arbor, MI, United States
PATENT ASSIGNEE(S):        Warner-Lambert Company, Morris Plains, NJ, United
                           States (U.S. corporation)

                                NUMBER         KIND    DATE
                           ---------------- ------ --------
PATENT INFORMATION:        US 6696440          B1   20040224
                           WO 2000040235            20000713          <--
APPLICATION INFO.:         US 2001-889091           20010711  (9)
                           WO 1999-US30419          19991221

                                  NUMBER         DATE
                           ------------------ --------
PRIORITY INFORMATION:      US 1999-115086P    19990107 (60)
DOCUMENT TYPE:             Utility
FILE SEGMENT:              GRANTED
PRIMARY EXAMINER:          Spivack, Phyllis G.
ASSISTANT EXAMINER:        Delacroix-Muirheid, C.
LEGAL REPRESENTATIVE:      Shen, Evelyn D., Harvey, Suzanne M.
NUMBER OF CLAIMS:          13
EXEMPLARY CLAIM:           1
NUMBER OF DRAWINGS:        0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT:                2500
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB     This invention provides a method of preventing or treating asthma by
       administering to a patient in need of treatment an effective amount of a
       selective MEK inhibitor, especially a phenyl amine of Formula I and II:
       ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT   57381-34-7P, 5-Chloro-2-fluorobenzonitrile
       (prepn. of 2-(4-bromo or 4-iodo phenylamino)benzoic acid derivs. as MEK
       inhibitors by addn. of halobenzoic acids to haloanilines and optional
       redn. or amidation of the acid)
RN   57381-34-7  USPATFULL
CN   Benzonitrile, 5-chloro-2-fluoro- (9CI)  (CA INDEX NAME)
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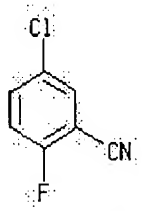


L27 ANSWER 2 OF 63 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:79134 USPATFULL
TITLE: 2,7-substituted octahydro-1H-pyrido[1,2-A]pyrazine derivatives as ligands for serotonin receptors
INVENTOR(S): Desai, Kishor A., Ledyard, CT, UNITED STATES
Fliri, Anton F., Stonington, CT, UNITED STATES
Sanner, Mark A., Old Saybrook, CT, UNITED STATES
PATENT ASSIGNEE(S): Pfizer Inc. (U.S. corporation)

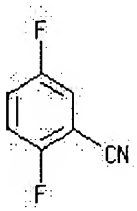
	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003055061	A1	20030320	<--
APPLICATION INFO.:	US 2002-213604	A1	20020807 (10)	

RELATED APPLN. INFO.: Continuation of Ser. No. US 2001-784567, filed on 15 Feb 2001, ABANDONED Continuation of Ser. No. US 1999-368984, filed on 5 Aug 1999, GRANTED, Pat. No. US 6231833 Continuation-in-part of Ser. No. US 1998-135946, filed on 18 Aug 1998, ABANDONED Continuation-in-part of Ser. No. US 1997-809145, filed on 26 Mar 1997, GRANTED, Pat. No. US 5852031 A 371 of International Ser. No. WO 1995-IB689, filed on 24 Aug 1995, UNKNOWN Continuation of Ser. No. US 1994-315470, filed on 30 Sep 1994, ABANDONED
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: PFIZER INC, 150 EAST 42ND STREET, 5TH FLOOR - STOP 49, NEW YORK, NY, 10017-5612
NUMBER OF CLAIMS: 1
EXEMPLARY CLAIM: 1
LINE COUNT: 2406
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Substituted pyrido[1,2-a]pyrazines of general formula I; wherein Ar and Ar^1 represent various carbocyclic and heterocyclic aromatic rings; A represents O, S, SO, SO_2, CHOH, C.dbd.O, or --(CR^{3R4}); and n is 0-2, as well as precursors thereto, are ligands for dopamine receptor subtypes and serotonin (5HT) within the body and are therefore useful in the treatment of disorders of the dopamine and serotonin systems: ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **64248-64-2**, 2,5-Difluorobenzonitrile
(prepn. of N-aryloctahydro-1H-pyrido[1,2-a]pyrazines as dopamine receptor ligands)
RN 64248-64-2 USPATFULL
CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



L27 ANSWER 3 OF 63 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:79133 USPATFULL
TITLE: Imidazo-triazine derivatives as ligands for GABA receptors
INVENTOR(S): Carling, William Robert, Bishops Stortford, UNITED KINGDOM
Hallett, David James, Watford, UNITED KINGDOM
Russell, Michael Geoffrey Neil, Welwyn Garden City, UNITED KINGDOM
Street, Leslie Joseph, Little Hallingbury, UNITED KINGDOM

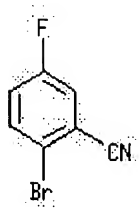
	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003055060	A1	20030320	<--
	US 6617326	B2	20030909	
APPLICATION INFO.:	US 2002-195274	A1	20020715	(10)

	NUMBER	DATE
PRIORITY INFORMATION:	GB 2001-17277	20010716

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MERCK AND CO INC, P O BOX 2000, RAHWAY, NJ, 070650907
NUMBER OF CLAIMS: 10
EXEMPLARY CLAIM: 1
LINE COUNT: 1172
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A class of 7-phenylimidazo[1,2-b][1,2,4]triazine derivatives, substituted at the meta position of the phenyl ring by a (cyano)(fluoro)phenyl moiety, being selective ligands for $GABA_A$ receptors, in particular having good affinity for the α2 and/or α3 subunit thereof, are accordingly of benefit in the treatment and/or prevention of adverse conditions of the central nervous system, including anxiety and convulsions.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **57381-39-2**, 2-Bromo-5-fluorobenzonitrile
(prepn. of imidazo-triazines as ligands for GABA receptors)
RN 57381-39-2 USPATFULL
CN Benzonitrile, 2-bromo-5-fluoro- (9CI) (CA INDEX NAME)



h eb c g cg b cg eb

L27 ANSWER 4 OF 63 USPATFULL on STN

Full Text | Claims References

ACCESSION NUMBER: 2003:72001 USPATFULL
TITLE: Cyclic regimens utilizing indoline derivatives
INVENTOR(S): Grubb, Gary S., Newtown Square, PA, UNITED STATES
Fensome, Andrew, Wayne, PA, UNITED STATES
Miller, Lori L., Wayne, PA, UNITED STATES
Ullrich, John W., Exton, PA, UNITED STATES
Bender, Reinhold H.W., Valley Forge, PA, UNITED STATES
Zhang, Puwen, Audubon, PA, UNITED STATES
Wrobel, Jay E., Lawrenceville, NJ, UNITED STATES
Edwards, James P., San Diego, CA, UNITED STATES
Jones, Todd K., Solana Beach, CA, UNITED STATES
Tegley, Christopher M., Thousand Oaks, CA, UNITED STATES
Zhi, Lin, San Diego, CA, UNITED STATES
PATENT ASSIGNEE(S): WYETH, Madison, NJ (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003050288	A1	20030313	<--
	US 6544970	B2	20030408	
APPLICATION INFO.:	US 2002-153393	A1	20020522 (10)	

RELATED APPLN. INFO.: Division of Ser. No. US 2000-552358, filed on 19 Apr 2000, PENDING

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183052P	19990504 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: HOWSON AND HOWSON, ONE SPRING HOUSE CORPORATION CENTER, BOX 457, 321 NORRISTOWN ROAD, SPRING HOUSE, PA, 19477
NUMBER OF CLAIMS: 25
EXEMPLARY CLAIM: 1
LINE COUNT: 4003
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure: ##STR1##

wherein R_1 and R_2 may be single substituents or fused to form spirocyclic rings, in combination with progestins, estrogens, or both. These methods of treatment may be used for contraception, for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis, polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, or prostate, minimization of side effects, cyclic menstrual bleeding, or stimulation of food intake.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **179897-89-3**
(prepn. of oxospiro[cycloalkane-1,3'-indoline] derivs. and analogs as progesterone receptor antagonists)
RN 179897-89-3 USPATFULL
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)

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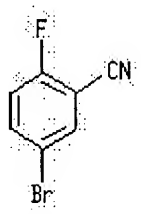


L27 ANSWER 5 OF 63 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:65387 USPATFULL
TITLE: Combination regimens using progesterone receptor modulators
INVENTOR(S): Grubb, Gary S., Newtown Square, PA, UNITED STATES
Zhang, Puwen, Audubon, PA, UNITED STATES
Terefenko, Eugene A., Quakertown, PA, UNITED STATES
Fensome, Andrew, Wayne, PA, UNITED STATES
Wrobel, Jay E., Lawrenceville, NJ, UNITED STATES
Fletcher, Horace, III, Pottstown, PA, UNITED STATES
Edwards, James P., San Diego, CA, UNITED STATES
Jones, Todd K., Solana Beach, CA, UNITED STATES
Tegley, Christopher M., Thousand Oaks, CA, UNITED STATES
Zhi, Lin, San Diego, CA, UNITED STATES
PATENT ASSIGNEE(S): WYETH, Madison, NJ (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003045511	A1	20030306	<--
	US 6759408	B2	20040706	
APPLICATION INFO.:	US 2002-141792	A1	20020509 (10)	

RELATED APPLN. INFO.: Division of Ser. No. US 2000-552350, filed on 19 Apr 2000, PENDING

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-229346P	19990504 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: HOWSON AND HOWSON, ONE SPRING HOUSE CORPORATION CENTER, BOX 457, 321 NORRISTOWN ROAD, SPRING HOUSE, PA, 19477
NUMBER OF CLAIMS: 29
EXEMPLARY CLAIM: 1
LINE COUNT: 4295
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

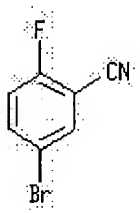
AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure: ##STR1##

wherein R^1 and R^2 may be single substituents or fused; R^3 is H, OH, NH_2, C_1 to C_6 alkyl, COR^C, or optionally substituted C_1 to C_6 alkyl, C_3 to C_6 alkenyl, or alkynyl; R^C is H, or optionally substituted C_1 to C_3 alkyl, aryl, C_1 to C_3 alkoxy, or C_1 to C_3 aminoalkyl; R^4 is H, halogen, CN, NO_2, or optionally substituted C_1 to C_6 alkyl, alkynyl, C_1 to C_6

h eb c g cg b cg eb

alkoxy, amino, or C_1 to C_6 aminoalkyl; and R^5 is a benzene ring, a five or six membered heterocyclic ring; or pharmaceutically acceptable salt thereof. Methods of treatment include contraception, secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis, polycystic ovary syndrome, carcinomas, adenocarcinomas minimization of side effects, or food intake stimulation.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **179897-89-3**
(prepn. of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)
RN 179897-89-3 USPATFULL
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004
L4 0 S L3/THU
L5 27 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004
E PYRIDINIUM ION/CN
L6 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004
L7 99 S L6/RCT
L8 0 S L7 AND L5
L9 717 S L6
L10 0 S L9 AND L5

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004
L11 STRUCTURE UPLOADED
L12 16 S L11
L13 2489 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004
L14 4838 S L13
L15 1 S L14 AND BOICE, G?/AU
L16 4837 S L14 NOT L15
L17 0 S L16 AND CONRAD, K?/AU
L18 0 S L16 AND CORLEY, E?/AU
L19 0 S L16 AND MATTY, L?/AU

h eb c g cg b cg eb

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L20             0 S L16 AND MURRY, J?/AU
L21             0 S L16 AND SAVARIN, C?/AU

     FILE 'REGISTRY' ENTERED AT 14:19:45 ON 01 OCT 2004
L22               STRUCTURE UPLOADED
L23             0 S L22
L24            24 S L22 FULL

     FILE 'HCAPLUS' ENTERED AT 14:20:39 ON 01 OCT 2004
L25           206 S L24

     FILE 'USPATFULL' ENTERED AT 14:21:07 ON 01 OCT 2004
L26            99 S L24
L27            63 S L26 AND PD < APRIL 2003

=> s 126 and pd < march 2003
       3405359 PD < MARCH 2003
                 (PD<20030300)
L28           59 L26 AND PD < MARCH 2003

=> d l28, ibib abs fhitstr, 1-10

L28  ANSWER 1 OF 59  USPATFULL on STN
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Full Text | Citing References

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ACCESSION NUMBER:         2004:46802  USPATFULL
TITLE:                    Treatment of asthma with MEK inhibitors
INVENTOR(S):              Bridges, Alexander James, Saline, MI, United States
                          Dudley, David Thomas, Ann Arbor, MI, United States
                          Mobley, James Leslie, Brighton, MI, United States
                          Saltiel, Alan Robert, Ann Arbor, MI, United States
PATENT ASSIGNEE(S):       Warner-Lambert Company, Morris Plains, NJ, United
                          States (U.S. corporation)

                               NUMBER         KIND    DATE
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PATENT INFORMATION:       US 6696440          B1   20040224
                          WO 2000040235            20000713          <--
APPLICATION INFO.:        US 2001-889091           20010711  (9)
                          WO 1999-US30419          19991221

                                 NUMBER         DATE
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PRIORITY INFORMATION:     US 1999-115086P    19990107 (60)
DOCUMENT TYPE:            Utility
FILE SEGMENT:             GRANTED
PRIMARY EXAMINER:         Spivack, Phyllis G.
ASSISTANT EXAMINER:       Delacroix-Muirheid, C.
LEGAL REPRESENTATIVE:     Shen, Evelyn D., Harvey, Suzanne M.
NUMBER OF CLAIMS:         13
EXEMPLARY CLAIM:          1
NUMBER OF DRAWINGS:       0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT:               2500
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB     This invention provides a method of preventing or treating asthma by
       administering to a patient in need of treatment an effective amount of a
       selective MEK inhibitor, especially a phenyl amine of Formula I and II:
       ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
```
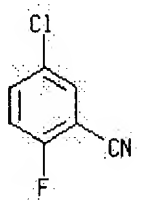

h eb c g cg b cg eb

IT **57381-34-7P**, 5-Chloro-2-fluorobenzonitrile
(prepn. of 2-(4-bromo or 4-iodo phenylamino)benzoic acid derivs. as MEK inhibitors by addn. of halobenzoic acids to haloanilines and optional redn. or amidation of the acid)
RN 57381-34-7 USPATFULL
CN Benzonitrile, 5-chloro-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 59 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:40676 USPATFULL
TITLE: 1-substituted phenyl-1-(1h-imidazol-4-yl) alcohols, process for producing the same and use thereof
INVENTOR(S): Tasaka, Akihiro, Suita, JAPAN
Kaku, Tomohiro, Nishinomiya, JAPAN
Kusaka, Masami, Kobe, JAPAN
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Osaka, JAPAN (non-U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6518257	B1	20030211	<--
	WO 2001030764		20010503	<--
APPLICATION INFO.:	US 2002-111136		20020418	(10)
	WO 2000-JP7284		20001019	

	NUMBER	DATE
PRIORITY INFORMATION:	JP 1999-301562	19991022

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Stockton, Laura L.
LEGAL REPRESENTATIVE: Chao, Mark, Ramesh, Elaine M.
NUMBER OF CLAIMS: 14
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT: 3893
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

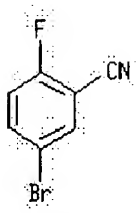
AB To provide a composition having a steroid C_{17},20-lyase inhibitory activity and useful as an agent for the prophylaxis or treatment of prostatism and tumors such as breast cancer. A compound represented by the formula: ##STR1##

wherein R is a hydrogen atom or a protecting group, R^1 is a lower alkyl group or a cyclic hydrocarbon group, R^2 is an aromatic hydrocarbon group optionally having substituents or an aromatic heterocyclic group optionally having substituents, R^3 is a hydrocarbon group optionally having substituents, a hydroxyl group optionally having substituents, a thiol group optionally having substituents, an amino group optionally having substituents, an acyl group or a halogen atom, and n is an integer of 0 to 4, and a salt

h eb c g cg b cg eb

thereof have a steroid C_{17},20-lyase inhibitory activity, and are useful as an agent for the pophylaxis or treatment of prostatism and tumors such as beast cancer and the like.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **179897-89-3**, 5-Bromo-2-fluorobenzonitrile
(prepn. process and use of phenylimidazolyl alcs. as antitumor agents)
RN 179897-89-3 USPATFULL
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 3 OF 59 USPATFULL on STN
Full Text | Citing References

ACCESSION NUMBER:	2003:20225 USPATFULL
TITLE:	Cyclocarbamate derivatives as progesterone receptor modulators
INVENTOR(S):	Zhang, Puwen, Audubon, PA, United States Terefenko, Eugene A., Quakertown, PA, United States Fensome, Andrew, Wayne, PA, United States Wrobel, Jay E., Lawrenceville, NJ, United States Fletcher, III, Horace, Pottstown, PA, United States Zhi, Lin, San Diego, CA, United States Jones, Todd K., Solana Beach, CA, United States Edwards, James P., San Diego, CA, United States Tegley, Christopher M., Thousand Oaks, CA, United States
PATENT ASSIGNEE(S):	American Home Products Corporation, Madison, NJ, United States (U.S. corporation) Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6509334	B1	20030121	<--
APPLICATION INFO.:	US 2000-552633		20000419 (9)	

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183012P	19990504 (60)

DOCUMENT TYPE:	Utility
FILE SEGMENT:	GRANTED
PRIMARY EXAMINER:	Ford, John M.
LEGAL REPRESENTATIVE:	Howson and Howson
NUMBER OF CLAIMS:	94
EXEMPLARY CLAIM:	1
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT:	4304

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention provides compounds of Formula (I): ##STR1##

wherein R^1 and R^2 may be single substituents or fused to form

h eb c g cg b cg eb

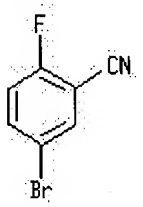
spirocyclic or hetero-spirocyclic rings; R^3 is H, OH, NH_2, C_1 to C_6 alkyl, substituted C_1 to C_6 alkyl, C_3 to C_6 alkenyl, substituted C_1 to C_6 alkenyl, alkynyl, or substituted alkynyl, COR^C; R^C is H, C_1 to C_3 alkyl, substituted C_1 to C_3 alkyl, aryl, substituted aryl, C_1 to C_3 alkoxy, substituted C_1 to C_3 alkoxy, C_1 to C_3 aminoalkyl, or substituted C_1 to C_3 aminoalkyl; R^4 is H, halogen, CN, NO_2, C_1 to C_6 alkyl, substituted C_1 to C_6 alkyl, alkynyl, or substituted alkynyl, C_1 to C_6 alkoxy, substituted C_1 to C_6 alkoxy, amino, C_1 to C_6 aminoalkyl, or substituted C_1 to C_6 aminoalkyl; and R^5 is selected from a trisubstituted benzene ring of a five or six membered ring with 1, 2, or 3 heteroatoms from the group including O, S, SO, SO_2 or NR^6 and containing one or two independent substituents from the group including H, halogen, CN, NO_2, amino, and C_1 to C_3 alkyl, C_1 to C_3 alkoxy, C_1 to C_3 aminoalkyl, COR^F, or NR^{GCORF}; or pharmaceutically acceptable salt thereof, as well as pharmaceutical compositions and methods using the compounds as antagonists of the progesterone receptor.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **179897-89-3**
(prepn. of benzooxazinone derivs. as progesterone receptor modulators)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 4 OF 59 USPATFULL on STN

Full Text | Claims | References

ACCESSION NUMBER: 2002:340320 USPATFULL

TITLE: Cyclic regimens using quinazolinone and benzoxazine derivatives

INVENTOR(S): Grubb, Gary S., Newtown Square, PA, United States
Zhi, Lin, San Diego, CA, United States
Jones, Todd K., Solana Beach, CA, United States
Zhang, Puwen, Audubon, PA, United States
Edwards, James P., San Diego, CA, United States
Fensome, Andrew, Wayne, PA, United States
Terefenko, Eugene A., Quakertown, PA, United States
Wrobel, Jay E., Lawrenceville, NJ, United States
Tegley, Christopher M., Thousand Oaks, CA, United States

PATENT ASSIGNEE(S): Wyeth, Madison, NJ, United States (U.S. corporation)
Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

	NUMBER	KIND	DATE

h eb c g cg b cg eb

PATENT INFORMATION:	US 6498154	B1	20021224 <--
APPLICATION INFO.:	US 2000-552357		20000419 (9)

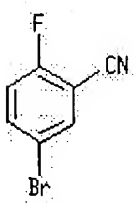
	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183042P	19990504 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Travers, Russell
ASSISTANT EXAMINER: Hui, San-ming
LEGAL REPRESENTATIVE: Howson and Howson
NUMBER OF CLAIMS: 17
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT: 2607
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies utilizing, in combination with progestins, estrogens, or both, compounds which are progesterone receptor antagonists of the general structure: ##STR1##

wherein: R^1 and R^2 are H, COR^A, or NR^{BCORA}, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, or heterocyclic; or R^1 and R^2 fuse to form 3 to 8 membered spirocyclic alkyl, alkenyl or heterocyclic rings; R^A is H or optionally substituted alkyl, aryl, alkoxy, or aminoalkyl groups; R^B is H or alkyl; R^3 is H, OH, NH_2, COR^C or alkyl, alkenyl, or alkynyl; R^C is H, alkyl, aryl, alkoxy, or aminoalkyl; R^4 is H, halogen, CN, NO_2, alkyl, alkynyl, alkoxy, amino or aminoalkyl; R^5 is benzene or 5- or 6-membered heterocyclic ring; R^6 is H or alkyl; G_1 is O, NR_7, or CR_{7R8}; G_2 is CO or CR_{7R8}; provided that when G_1 is O, G_2 is CR_{7R8}, and G_1 and G_2 cannot both be CR_{7R8}; R_7 and R_8 are H or an optionally substituted alkyl, aryl, or heterocyclic moiety; or pharmaceutically acceptable salt thereof. These methods may be used for contraception or treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects or cyclic menstrual bleeding. Additional uses of the invention include stimulation of food intake.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **179897-89-3**
(prepn. of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)
RN 179897-89-3 USPATFULL
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



h eb c g cg b cg eb

L28 ANSWER 5 OF 59 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:338031 USPATFULL
TITLE: Thrombin inhibitors
INVENTOR(S): Barrow, James C., Harleysville, PA, UNITED STATES
Coburn, Craig, Royersford, PA, UNITED STATES
Selnick, Harold G., Ambler, PA, UNITED STATES
Ngo, Phung L., Upper Darby, PA, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002193398	A1	20021219	<--
	US 6610701	B2	20030826	
APPLICATION INFO.:	US 2002-71422	A1	20020208	(10)

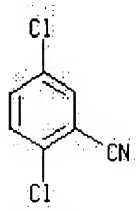
	NUMBER	DATE
PRIORITY INFORMATION:	US 2001-267960P	20010209 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MERCK AND CO INC, P O BOX 2000, RAHWAY, NJ, 070650907
NUMBER OF CLAIMS: 21
EXEMPLARY CLAIM: 1
LINE COUNT: 2878
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compounds of the invention are useful in inhibiting thrombin and treating blood coagulation and cardiovascular disorders and have the following structure: ##STR1##

wherein

R^3 is hydrogen or halogen, and u is N or CH.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **21663-61-6**, 2,5-Dichlorobenzonitrile
(prepn. of 2-(pyridin-4-yl)acetamides as thrombin inhibitors)
RN 21663-61-6 USPATFULL
CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 6 OF 59 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:280635 USPATFULL
TITLE: Pyrazolopyrimidines as therapeutic agents
INVENTOR(S): Hirst, Gavin C., Marlborough, MA, UNITED STATES
Rafferty, Paul, Westborough, MA, UNITED STATES
Ritter, Kurt, Newton, GERMANY, FEDERAL REPUBLIC OF
Calderwood, David, Framingham, UNITED KINGDOM
Wishart, Neil, Jefferson, MA, UNITED STATES
Arnold, Lee D., Westborough, CANADA

h eb c g cg b cg eb

	Friedman, Michael M., Newton, MA, UNITED STATES
PATENT ASSIGNEE(S):	Abbott Laboratories, Abbott Park, IL, UNITED STATES (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002156081	A1	20021024	<--
APPLICATION INFO.:	US 2001-815310	A1	20010322	(9)

RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 2000-663780, filed on 15 Sep 2000, PENDING

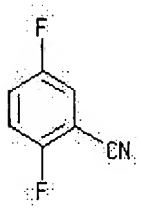
	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-154620P	19990917 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: LAHIVE & COCKFIELD, 28 STATE STREET, BOSTON, MA, 02109
NUMBER OF CLAIMS: 138
EXEMPLARY CLAIM: 1
LINE COUNT: 30126
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides compounds of Formula I, ##STR1##

including pharmaceutically acceptable salts and/or prodrugs thereof, where G, R_2, and R_3 are defined as described herein.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **64248-64-2**, 2,5-Difluorobenzonitrile
(prepn. of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)
RN 64248-64-2 USPATFULL
CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 7 OF 59 USPATFULL on STN

Full Text | CITED References

ACCESSION NUMBER:	2002:262352 USPATFULL
TITLE:	Cyclic regimens utilizing indoline derivatives
INVENTOR(S):	Grubb, Gary S., Newtown Square, PA, United States Fensome, Andrew, Wayne, PA, United States Miller, Lori L., Wayne, PA, United States Ullrich, John W., Exton, PA, United States Bender, Reinhold H. W., Valley Forge, PA, United States Zhang, Puwen, Audubon, PA, United States Wrobel, Jay E., Lawrenceville, NJ, United States Edwards, James P., San Diego, CA, United States Jones, Todd K., Solana Beach, CA, United States Tegley, Christopher M., Thousand Oaks, CA, United States Zhi, Lin, San Diego, CA, United States
PATENT ASSIGNEE(S):	Wyeth, Madison, NJ, United States (U.S. corporation)

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Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6462032	B1	20021008	<--
APPLICATION INFO.:	US 2000-552358		20000419 (9)	

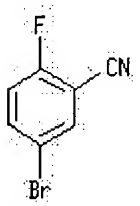
	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183052P	19990504 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Travers, Russell
ASSISTANT EXAMINER: Hui, San-ming
LEGAL REPRESENTATIVE: Howson and Howson
NUMBER OF CLAIMS: 16
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT: 3730
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure:
##STR1##

wherein R^1 and R^2 may be single substituents or fused to form spirocyclic rings, in combination with progestins, estrogens, or both. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects or cyclic menstrual bleeding. Additional uses of the invention include stimulation of food intake.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **179897-89-3**
(prepn. of oxospiro[cycloalkane-1,3'-indoline] derivs. and analogs as progesterone receptor antagonists)
RN 179897-89-3 USPATFULL
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 8 OF 59 USPATFULL on STN

Full Text | Chng References

ACCESSION NUMBER: 2002:259430 USPATFULL
TITLE: Monoamine reuptake inhibitors for treatment of CNS disorders
INVENTOR(S): Howard, Harry R., JR., Bristol, CT, UNITED STATES
Schmidt, Christopher J., Old Lyme, CT, UNITED STATES
Seeger, Thomas F., Mystic, CT, UNITED STATES

h eb c g cg b cg eb

Elliott, Mark L., Canterbury, CT, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002143003	A1	20021003	<--
	US 6677378	B2	20040113	
APPLICATION INFO.:	US 2001-845992	A1	20010430 (9)	

RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 529207, PENDING A 371 of International Ser. No. WO 2000-IB108, filed on 2 Feb 2000, UNKNOWN

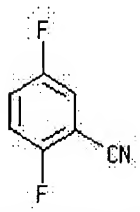
	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-121313P	19990223 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: Paul H. Ginsburg, Pfizer Inc., 20th Floor, 235 East 42nd Street, New York, NY, 10017-5755
NUMBER OF CLAIMS: 15
EXEMPLARY CLAIM: 1
LINE COUNT: 1999
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to compounds of the formula ##STR1##

wherein R^1 through R^4, X, Y, m and n are defined as in the specification. Such compounds are useful exhibit activity as serotonin, norepinephrine and dopamine reuptake inhibitors, and their pharmaceutically acceptable salts, and their use in the treatment of central nervous system and other disorders.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **64248-64-2**, 2,5-Difluorobenzonitrile
(prepn. of phenoxybenzylamines as monoamine reuptake inhibitors)
RN 64248-64-2 USPATFULL
CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 9 OF 59 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:243620 USPATFULL
TITLE: 2,7-substituted octahydro-1H-pyrido[1,2-A]pyrazine derivatives as ligands for serotonin receptors
INVENTOR(S): Desai, Kishor A., Ledyard, CT, UNITED STATES
Fliri, Anton F., Stonington, CT, UNITED STATES
Sanner, Mark A., Old Saybrook, CT, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002132811	A1	20020919	<--
APPLICATION INFO.:	US 2001-784567	A1	20010215 (9)	

RELATED APPLN. INFO.: Continuation of Ser. No. US 1999-368984, filed on 5 Aug

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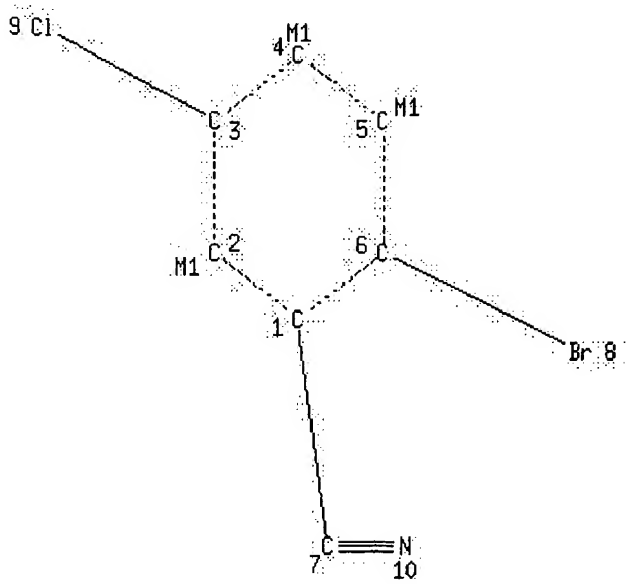


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HCOUNT   IS M1      AT    4
HCOUNT   IS M1      AT    5
NSPEC    IS R       AT    1
NSPEC    IS R       AT    2
NSPEC    IS R       AT    3
NSPEC    IS R       AT    4
NSPEC    IS R       AT    5
NSPEC    IS R       AT    6
NSPEC    IS C       AT    7
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NSPEC    IS C       AT    9
NSPEC    IS C       AT   10
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS   AT    7  8  9 10
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE


=> s 129
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SAMPLE SCREEN SEARCH COMPLETED -     13 TO ITERATE

100.0% PROCESSED      13 ITERATIONS                          1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           44 TO      476
PROJECTED ANSWERS:               1 TO       80

L30           1 SEA SSS SAM L29

=> s 129 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS


h        eb c     g cg  b     cg                              eb
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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:24:03 FILE 'REGISTRY'
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100.0% PROCESSED     295 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

L31           1 SEA SSS FUL L29

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FULL ESTIMATED COST                                      155.84     834.15

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CA SUBSCRIBER PRICE                                        0.00     -14.70

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FILE COVERS 1907 - 1 Oct 2004  VOL 141 ISS 15
FILE LAST UPDATED: 30 Sep 2004  (20040930/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l31
L32           4 L31

=> d l32, ibib abs fhitstr, 1-4

L32  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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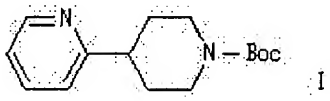
ACCESSION NUMBER:         2004:511300  HCAPLUS
DOCUMENT NUMBER:          141:174054
TITLE:                    Direct synthesis of 4-arylpiperidines via
                          palladium/copper(I)-cocatalyzed Negishi coupling of a
                          4-piperidylzinc iodide with aromatic halides and
                          triflates
AUTHOR(S):                Corley, Edward G.; Conrad, Karen; Murry, Jerry A.;
                          Savarin, Cecile; Holko, Justin; Boice, Genevieve
CORPORATE SOURCE:         Departments of Process Research, and Chemical
                          Engineering Research & Development, Merck Research
                          Laboratories, Merck and Co., Inc., Rahway, NJ, 07065,
```

h eb c g cg b cg eb

USA
SOURCE: Journal of Organic Chemistry (2004), 69(15), 5120-5123
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

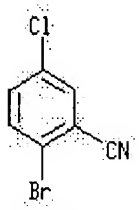


I

AB A general procedure for the synthesis of 4-arylpiperidines, e.g., I, via the coupling of 4-(N-Boc-piperidyl)zinc iodide with aryl halides and triflates is presented. The reaction required cocatalysis with both Cl2Pd(dppf) and a copper(I) species. An improved, safer procedure for the activation of zinc dust is also presented.

IT **57381-37-0**, 2-Bromo-5-chlorobenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-(Boc)-arylpiperidines via addn. of zinc to N-(Boc)-iodopiperidine followed by palladium/copper-catalzyed Negishi coupling with aryl halides and triflates)

RN 57381-37-0 HCAPLUS
CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:736258 HCAPLUS
DOCUMENT NUMBER: 137:263048
TITLE: Imidazo-pyrimidine derivatives as ligands for GABA receptors, and their preparation, pharmaceutical compositions, and use in the treatment of adverse neurological conditions.
INVENTOR(S): Chambers, Mark Stuart; Goodacre, Simon Charles; Hallett, David James; Jennings, Andrew; Jones, Philip; Lewis, Richard Thomas; Moore, Kevin William; Russell, Michael Geoffrey Neil; Street, Leslie Joseph; Szekeres, Helen Jane
PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK
SOURCE: PCT Int. Appl., 197 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

h eb c g cg b cg eb

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002074773	A1	20020926	WO 2002-GB1352	20020319
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002193385	A1	20021219	US 2002-100797	20020319
EP 1381606	A1	20040121	EP 2002-706976	20020319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.:

GB 2001-7134	A	20010321
GB 2001-27938	A	20011121
US 2000-719712	A3	20001215
WO 2002-GB1352	W	20020319

OTHER SOURCE(S): MARPAT 137:263048

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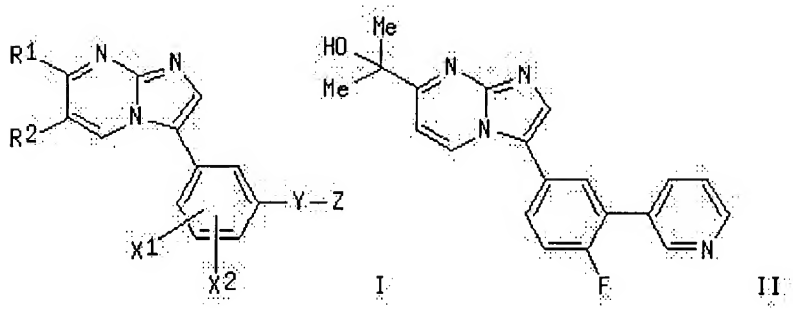
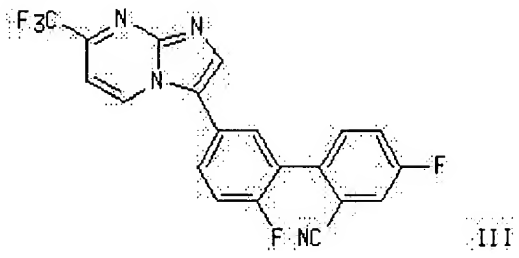




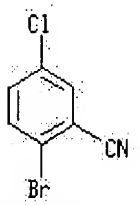
AB A class of 3-phenylimidazo[1,2-a]pyrimidine derivs. is disclosed. The compds. are substituted at the meta position of the Ph ring by an optionally substituted aryl or heteroaryl group, which is directly attached or bridged by an oxygen atom or an amino (NH) linkage, and which are further substituted on the Ph ring by alkyl, CF3, alkoxy, or one or two halogen atoms, esp. fluoro. The compds. are selective ligands for GABAA receptors, in particular having good affinity for the α2 and/or α3 and/or α5 subunit thereof, and are accordingly of benefit in the treatment and/or prevention of adverse conditions of the central nervous system, including anxiety, convulsions, and cognitive disorders. In particular, the compds. are represented by I [wherein X1 = halo, C1-6 alkyl, CF3, or C1-6 alkoxy; X2 = H or halo; Y = bond, O, or NH;

h eb c g cg b cg eb

Z = (un)substituted aryl or heteroaryl; R1 = H, hydrocarbyl, heterocyclyl, halo, cyano, CF3, NO2, ORa, SRa, SORa, SO2Ra, SO2NRaRb, NRaRb, NRaCORb, NRaCO2Rb, CORa, CO2Ra, CONRaRb, or CRa:NORb; R2 = H or halo; Ra, Rb = H, hydrocarbyl, or heterocyclyl], and include their salts and prodrugs. For instance, 3-hydroxy-3-methyl-2-butanone was O-acetylated, condensed with tri-Et orthoformate, and then cyclocondensed with 2-aminoimidazole hemisulfate to give 2-(imidazo[1,2-a]pyrimidin-7-yl)propan-2-ol. This compd. underwent ring bromination in the 3-position, followed by Pd(0)-catalyzed coupling of the bromide with 3-[2-fluoro-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)phenyl]pyridine, to give preferred title compd. II, isolated as the di-HCl salt. Another preferred compd., III, was prepd. via coupling of 3-bromo-7-trifluoromethylimidazo[1,2-a]pyrimidine with 5'-(5,5-dimethyl-[1,3,2]dioxaborinan-2-yl)-4,2'-difluorobiphenyl-2-carbonitrile (prepns. given). I potently inhibited the binding of [3H]-flumazenil to the benzodiazepine binding site of human GABAA receptors contg. α2 and/or α3 and/or α5 subunits (stably expressed in Ltk- cells), with all example compds. showing a Ki of 100 nM or less.

IT **57381-37-0P**, 2-Bromo-5-chlorobenzonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of imidazopyrimidine derivs. as GABAA receptor ligands for use as anxiolytics, anticonvulsants, and cognition enhancers)

RN 57381-37-0 HCAPLUS
CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1992:59379 HCAPLUS
DOCUMENT NUMBER: 116:59379
TITLE: Preparation of 4-(tetrazolylbiphenylylmethoxy)pyridines and related compounds as angiotensin II antagonists
INVENTOR(S): Roberts, David Anthony; Bradbury, Robert Hugh; Ratcliffe, Arnold Harry
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Eur. Pat. Appl., 55 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 453210	A2	19911023	EP 1991-303300	19910415
EP 453210	A3	19930113		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

h eb c g cg b cg eb

GB 2244054	A1	19911120	GB 1991-8081		19910415
GB 2244054	B2	19940406			
CA 2040747	AA	19911020	CA 1991-2040747		19910418
NO 9101534	A	19911021	NO 1991-1534		19910418
AU 9175083	A1	19911024	AU 1991-75083		19910418
ZA 9102912	A	19911224	ZA 1991-2912		19910418
US 5130318	A	19920714	US 1991-687270		19910418
JP 06199796	A2	19940719	JP 1991-228211		19910418
JP 3120873	B2	20001225			
FI 9101924	A	19911020	FI 1991-1924		19910419
CN 1055925	A	19911106	CN 1991-102514		19910419
HU 57206	A2	19911128	HU 1991-1295		19910419
US 5198439	A	19930330	US 1992-874785		19920427
PRIORITY APPLN. INFO.:			GB 1990-8817	A	19900419
			GB 1990-26617	A	19901207
			US 1991-687270	A3	19910418

OTHER SOURCE(S): MARPAT 116:59379
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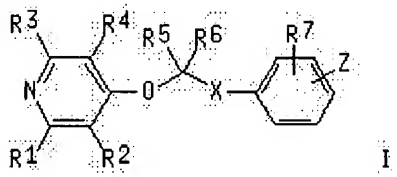

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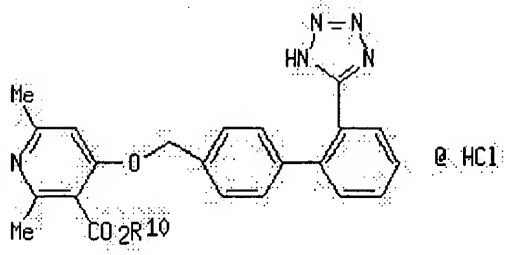

II

AB Title compds. [I; R1 = H, (cyclo)alkyl, Ph, substituted alkyl; R2 = H, (cyclo)alkyl, cycloalkylalkyl, CO2H, alkoxycarbonyl, cyano, NO2, Ph, phenylalkyl; R3 = halo, alkoxy, amino, R1; R4 = H, (substituted) alkyl, carboxy, alkoxycarbonyl, cyano, NO2, carbamoyl, halo, amino, acylamino, etc.; R3R4 = (CO-interrupted) alkylene, alkenylene; R5 = H; R6 = H, alkyl; R7 = R6, alkoxy, halo, CF3, cyano, NO2; X = (substituted) phenylene, bond; Z = tetrazolyl tetrazolylaminocarbonyl, etc.; and N-oxides thereof], were prepd. Thus, Et 1,4-dihydro-2,6-dimethyl-4-oxopyridine-3-carboxylate was condensed with 5-[2-(4'-bromomethylbiphenylyl)]-2-triphenylmethyl-2H-tetrazole using NaH in DMF and the product was detritylated with 6 M HCl in dioxane to give title compd. II (R10 = Et). II (R10 = Me) in rats antagonized angiotensin II with IC50 = 0.1 ms/kg i.v.

IT **57381-37-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for angiotensin II antagonists)

RN 57381-37-0 HCAPLUS
CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

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FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          119 TO      641
PROJECTED ANSWERS:               0 TO        0

L34           0 SEA SSS SAM L33

=> s l33 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
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FULL SEARCH INITIATED 14:26:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    461 TO ITERATE

100.0% PROCESSED     461 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.01

L35           1 SEA SSS FUL L33

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FULL ESTIMATED COST                               156.26    1011.81

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FILE COVERS 1907 - 1 Oct 2004  VOL 141 ISS 15
FILE LAST UPDATED: 30 Sep 2004  (20040930/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l35
L36           4 L35

=> d l36, ibib abs fhitstr, 1-4

L36  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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ACCESSION NUMBER:         2002:669675  HCAPLUS
DOCUMENT NUMBER:          137:201317
```

h ebc gcgb cg eb

TITLE: Preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents.

INVENTOR(S): Grubb, Gary S.; Zhang, Puwen; Terefenko, Eugene A.; Fensome, Andrew; Wrobel, Jay E.; Fletcher, Iii Horace; Edwards, James P.; Jones, Todd K.; Tegley, Christopher M.; Zhi, Lin

PATENT ASSIGNEE(S): Wyeth, John and Brother Ltd., USA; Ligand Pharmaceuticals Incorporated

SOURCE: U.S., 44 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6444668	B1	20020903	US 2000-552350	20000419
JP 2002543155	T2	20021217	JP 2000-615048	20000501
US 2003045511	A1	20030306	US 2002-141792	20020509
US 6759408	B2	20040706		

PRIORITY APPLN. INFO.:

US 1999-229346P	P	19990504
US 1999-304712	A	19990504
US 2000-552350	A	20000419
WO 2000-US11643	W	20000501

OTHER SOURCE(S): MARPAT 137:201317

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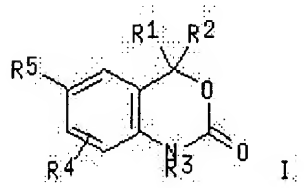

I

AB A method of contraception comprises administration to a female of a progestational agent in a first phase and in a second phase administration of [I; R1, R2 = H, (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, aryl, heterocyclyl, amino deriv.; R1R2 = atoms to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, C3-6 alkenyl, alkynyl, COR6; R6 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, alkynyl, C1-6 alkoxy, amino, C1-6 aminoalkyl; R5 = trisubstituted benzene ring, 5-6 membered ring with 1, 2, or 3 O, S, SO, SO2, NR7 and contg. 1-2 H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, NR9COR8; R7 = H, C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl]. Thus, 6-(3-chlorophenyl)-4,4-dimethyl-1,4-dihydrobenzo[d][1,3]-oxazin-2-one was prepd. from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. I demonstrated IC50's of 2.7-68 nM in a hPR decidualization assay.

IT **304854-55-5**, Benzonitrile, 3-bromo-5-chloro-
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

RN 304854-55-5 HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)

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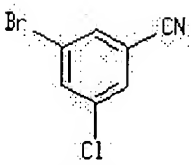

REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:790489 HCAPLUS
DOCUMENT NUMBER: 133:350229
TITLE: Novel cyclocarbamate derivatives as progesterone receptor modulators
INVENTOR(S): Zhang, Puwen; Terefenko, Eugene A.; Fletcher, Horace, III; Fensome, Andrew; Wrobel, Jay E.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066571	A1	20001109	WO 2000-US11822	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6509334	B1	20030121	US 2000-552633	20000419
EP 1173426	A1	20020123	EP 2000-928689	20000501
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BR 2000010213	A	20020219	BR 2000-10213	20000501
TR 200103286	T2	20020722	TR 2001-200103286	20000501
JP 2002543193	T2	20021217	JP 2000-615601	20000501
AU 766428	B2	20031016	AU 2000-46886	20000501
NZ 515355	A	20040227	NZ 2000-515355	20000501
US 2002049204	A1	20020425	US 2001-948309	20010906
US 6566358	B2	20030520		
ZA 2001007630	A	20020514	ZA 2001-7630	20010917
NO 2001005378	A	20020103	NO 2001-5378	20011102
BG 106079	A	20020531	BG 2001-106079	20011102
US 2003216388	A1	20031120	US 2003-386799	20030312
US 6713478	B2	20040330		
US 2004186101	A1	20040923	US 2004-767813	20040129
PRIORITY APPLN. INFO.:			US 1999-183012P	P 19990504

h eb c g cg b cg eb

US 2000-552633	A1	20000419
WO 2000-US11822	W	20000501
US 2001-948309	A3	20010906
US 2003-386799	A1	20030312

OTHER SOURCE(S): MARPAT 133:350229
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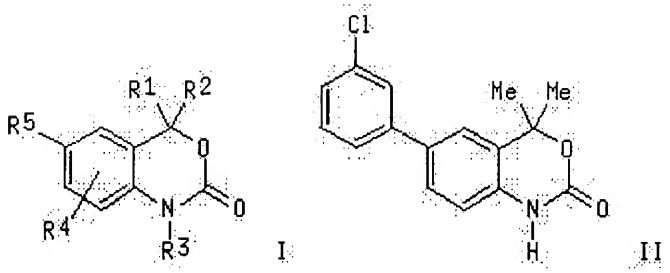
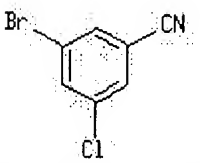


AB This invention discloses novel aryl fused cyclocarbamate derivs. I (R1 or R2 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, (un)substituted C3-8 cycloalkyl, (un)substituted aryl, (un)substituted heterocyclyl, amino deriv. or R1 and R2 may be fused to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, (un)substituted C3-6 alkenyl, (un)substituted alkynyl, or COR6 {R6 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy, or (un)substituted C1-3 aminoalkyl}; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, (un)substituted alkynyl, (un)substituted C1-6 alkoxy, amino, or (un)substituted C1-6 aminoalkyl; R5 = trisubstituted benzene ring or a five- or six-membered ring with 1, 2, or 3 heteroatoms selected from O, S, SO, SO2 or NR7 and contg. one or two independent substituents from the group including H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, or NR9COR8 {R7 = H or C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy or (un)substituted C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl}) or pharmaceutically acceptable salts thereof, as well as pharmaceutical compns. and methods using the compds. as antagonists of the progesterone receptor. Thus, cyclocarbamate II was prepd. from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. Compds. of the invention demonstrated potency in the range of 0.01 nM to 5 μM in the in vitro assays, and 0.001 to 300 mg/kg in the in vivo assays.

IT **304854-55-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of benzooxazinone derivs. as progesterone receptor modulators)

RN 304854-55-5 HCAPLUS
CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

h eb c g cg b cg eb

Full Text | Citing References

ACCESSION NUMBER: 2000:790488 HCAPLUS
DOCUMENT NUMBER: 133:350228
TITLE: Preparation of cyclothiocarbamate derivatives as progesterone receptor modulators
INVENTOR(S): Zhang, Puwen; Fensome, Andrew; Terefenko, Eugene A.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066570	A1	20001109	WO 2000-US11749	20000501
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EP 1175411	A1	20020130	EP 2000-930266	20000501
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TR 200103285	T2	20020221	TR 2001-200103285	20000501
JP 2002543192	T2	20021217	JP 2000-615600	20000501
AU 766801	B2	20031023	AU 2000-48119	20000501
CN 1131856	B	20031224	CN 2000-807099	20000501
NZ 515353	A	20040326	NZ 2000-515353	20000501
ZA 2001007633	A	20020514	ZA 2001-7633	20010917
NO 2001005381	A	20020103	NO 2001-5381	20011102
BG 106080	A	20020531	BG 2001-106080	20011102
US 2003092711	A1	20030515	US 2002-140034	20020506
PRIORITY APPLN. INFO.:			US 1999-183013P	P 19990504
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			WO 2000-US11749	W 20000501

OTHER SOURCE(S): MARPAT 133:350228
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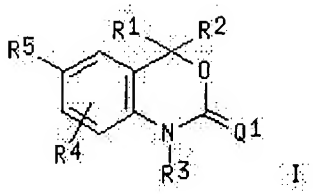

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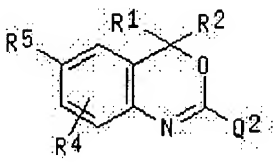


II

AB The title compds. [I or II; R1, R2 = H, alkyl, alkenyl, etc.; or R1 and R2 are fused to form (un)substituted 3-8 membered spiro cyclic alkyl or

h eb c g cg b cg eb

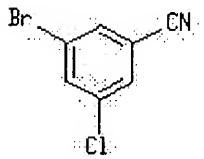
alkenyl ring or a spiro cyclic ring contg. 1-3 heteroatoms selected from O, S and N; R3 = H, OH, NH2, etc.; R4 = H, halo, CN, etc.; R5 = (un)substituted Ph, 5-6 membered heterocyclic ring with 1-3 ring heteroatoms, 3-pyridyl, 5-pyrimidinyl; Q1 = S, NR7, CR8R9; R7 = CN, alkyl, cycloalkyl, etc.; R8, R9 = H, alkyl, cycloalkyl, etc.; Q2 = NR11OR12, NR11NR12R13, ONR11R13; R11-R13 = H, alkyl, aryl, etc.] which are agonists of the progesterone receptor, and are useful for contraception and the treatment of progesterone-related maladies, were prepd. E.g., a multi-step synthesis of I [R1, R2 = Me; R3, R4 = H; R5 = 3-ClC6H4; Q1 = S] which showed EC50 of 0.65 nM against hPR in CV-1 cells, was given.

IT **304854-55-5**

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclothiocarbamate derivs. as progesterone receptor modulators)

RN 304854-55-5 HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:790347 HCAPLUS
DOCUMENT NUMBER: 133:350205
TITLE: Contraceptive compositions containing antiprogestinic and progestinic dihydro-2H-3,1-benzoxazin-2-ones
INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 146 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066164	A1	20001109	WO 2000-US11643	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6498154	B1	20021224	US 2000-552357	20000419
EP 1173210	A1	20020123	EP 2000-928611	20000501
EP 1173210	B1	20040915		

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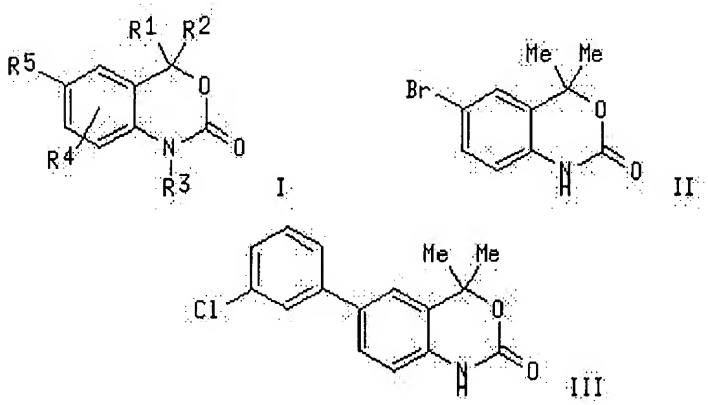
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

JP 2002543155 T2 20021217 JP 2000-615048 20000501
PRIORITY APPLN. INFO.: US 1999-304712 A 19990504
US 2000-552357 A1 20000419
US 1999-183042P P 19990504
US 2000-552350 A 20000419
WO 2000-US11643 W 20000501
OTHER SOURCE(S): MARPAT 133:350205

GI



AB The dihydrobenzoxazinones I [R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, acyl, acylamino; or R1R2 are fused to form spirocyclic or hetero-spirocyclic rings substituted by F, alkyl, alkoxy, alkylthio, F3C, HO, cyano, H2N, alkylamino; R3 = H, OH, NH2, C1-6 alkyl, C3-6 alkenyl, alkynyl, CORC; RC = H, C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, cyano, NO2, alkyl, alkynyl, alkoxy, alkoxy, amino, aminoalkyl; R5 = XYZC6H2, X = halo, cyano, alkyl, alkenyl, alkynyl, alkoxy, thioalkoxy, H2N, aminoalkyl, NO2, perfluoroalkyl, 5- or 6-membered heterocyclyl; Y, Z = H, halo, cyano, NO2, H2N, aminoalkyl, alkoxy, alkyl, thioalkoxy; or R5 = 5- or 6-membered heterocyclyl with O, S, SO, SO2 heteroatoms substituted by H, halo, cyano, NO2, H2N, alkyl, alkoxy, perfluoroacyl, perfluoroacylamino] and their pharmaceutically acceptable salts were prepd. as antagonists of the progesterone receptor and were useful to induce contraception in mammals in cyclic combination therapies using an antiprogestin and progestin where the progestin is administered in the alternating presence and absence of an antiprogestin. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects of cyclic menstrual bleeding. Addnl. uses of the invention include stimulation of food intake. Thus, cyclocondensation of 2-(2-amino-5-bromophenyl)-2-propanol with carbonyldiimidazole gave the dimethylbenzoxazinone II which coupled with 3-chlorophenylboronic acid in DME/H2O contg. (Ph3P)4Pd and Na2CO3 to give the (chlorophenyl)benzoxazinone III.

IT **304854-55-5**

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

RN 304854-55-5 HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)

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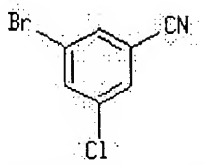

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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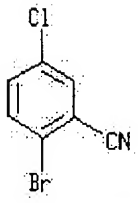

L32 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1975:606332 HCAPLUS
DOCUMENT NUMBER: 83:206332
TITLE: Benzoguanamine derivatives
INVENTOR(S): Murai, Hiromu; Ohata, Katsuya; Aoyagi, Yoshiaki; Ueda, Fusao; Kitano, Masahiko; Takata, Satoshi; Tada, Shinichi
PATENT ASSIGNEE(S): Nippon Shinyaku Co., Ltd., Japan
SOURCE: Ger. Offen., 24 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2506814	A1	19750828	DE 1975-2506814	19750218
DE 2506814	C3	19791115		
DE 2506814	B2	19790322		
JP 50111085	A2	19750901	JP 1974-19211	19740218
JP 55004751	B4	19800131		
JP 50111086	A2	19750901	JP 1974-19212	19740218
JP 52046955	B4	19771129		
US 3966728	A	19760629	US 1975-544176	19750127
CH 592639	A	19771031	CH 1975-1301	19750204
CH 592638	A	19771031	CH 1975-1300	19750204
SE 7501273	A	19750819	SE 1975-1273	19750205
SE 425245	B	19820913	SE 1975-1274	19750205
SE 425245	C	19821230		
DK 7500436	A	19751020	DK 1975-436	19750207
DK 138268	C	19790212		
DK 138116	B	19780717	DK 1975-437	19750207
DK 138116	C	19781204		
NL 7501574	A	19750820	NL 1975-1574	19750211
NL 157901	B	19780915		
NL 157902	B	19780915	NL 1975-1575	19750211
FR 2261009	A1	19750912	FR 1975-4690	19750214
BE 825673	A1	19750616	BE 1975-153471	19750218
AT 7501200	A	19770315	AT 1975-1200	19750218
AT 339909	B	19771110		
AT 7501197	A	19770515	AT 1975-1197	19750218
AT 340941	B	19780110		
PRIORITY APPLN. INFO.:			JP 1974-19211	19740218
			JP 1974-19212	19740218

GI For diagram(s), see printed CA Issue.

AB Triazines I (R = 2-Cl, 2-F, 2-Br, 3-Cl, R1 = 5-Cl; R = 2-Cl, R1 = 5-Br, 4-Cl, 3-Cl, 6-Cl, 5-F; R = 2-Br, 2-F, R1 = 5-F, 5-Br, 4-Cl; R = 3-Cl, R1 = 4-Br) were prepd. by treating RR1C6H3CN with dicyandiamide or dihalobenzoic acid derivs. with biguanide. I inhibit ulceration. Thus 20

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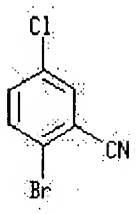
mg/kg I (R = 2-Cl, R1 = 5-Cl) i.p. in rats gave total inhibition of Shay ulcers.

IT **57381-37-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dicyanamide)

RN 57381-37-0 HCAPLUS
CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



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CA SUBSCRIBER PRICE	-2.80	-17.50

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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6
DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L33 STRUCTURE UPLOADED

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1999, GRANTED, Pat. No. US 6231833 Continuation-in-part of Ser. No. US 1998-135946, filed on 18 Aug 1998, ABANDONED Continuation-in-part of Ser. No. US 1997-809145, filed on 26 Mar 1997, GRANTED, Pat. No. US 5852031 Continuation-in-part of Ser. No. WO 1995-IB689, filed on 24 Aug 1995, UNKNOWN Continuation of Ser. No. US 1994-315470, filed on 30 Sep 1994, ABANDONED

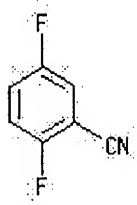
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: PFIZER INC, 150 EAST 42ND STREET, 5TH FLOOR - STOP 49, NEW YORK, NY, 10017-5612
NUMBER OF CLAIMS: 36
EXEMPLARY CLAIM: 1
LINE COUNT: 2614
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Substituted pyrido[1,2-a]pyrazines of general formula I; wherein Ar and Ar^1 represent various carbocyclic and heterocyclic aromatic rings; A represents O, S, SO, SO_2, CHOH, C.dbd.O, or --(CR^{3R4}); and n is 0-2, as well as precursors thereto, are ligands for dopamine receptor subtypes and serotonin (5HT) within the body and are therefore useful in the treatment of disorders of the dopamine and serotonin systems: ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **64248-64-2**, 2,5-Difluorobenzonitrile
(prepn. of N-aryloctahydro-1H-pyrido[1,2-a]pyrazines as dopamine receptor ligands)

RN 64248-64-2 USPATFULL
CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 10 OF 59 USPATFULL on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:224612 USPATFULL
TITLE: Combination regimens using progesterone receptor modulators
INVENTOR(S): Grubb, Gary S., Newtown Square, PA, United States
Zhang, Puwen, Audubon, PA, United States
Terefenko, Eugene A., Quakertown, PA, United States
Fensome, Andrew, Wayne, PA, United States
Wrobel, Jay E., Lawrenceville, NJ, United States
Fletcher, III, Horace, Pottstown, PA, United States
Edwards, James P., San Diego, CA, United States
Jones, Todd K., Solana Beach, CA, United States
Tegley, Christopher M., Thousand Oaks, CA, United States
Zhi, Lin, San Diego, CA, United States
PATENT ASSIGNEE(S): Wyeth, Madison, NJ, United States (U.S. corporation)
Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

h eb c g cg b cg eb

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6444668	B1	20020903	<--
APPLICATION INFO.:	US 2000-552350		20000419 (9)	

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-229346P	19990504 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Travers, Russell
ASSISTANT EXAMINER: Wang, Shengjun
LEGAL REPRESENTATIVE: Howson and Howson
NUMBER OF CLAIMS: 29
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT: 4086
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure: ##STR1##

wherein R^1 and R^2 may be single substituents or fused to form spirocyclic or hetero-spirocyclic rings; R^3 is H, OH, NH_2, C_1 to C_6 alkyl, substituted C_1 to C_6 allyl C_3 to C_6 alkenyl, substituted C_1 to C_6 alkenyl, alkynyl, or substituted alknyl, COR^C; R^C is H, C_1 to C_3 alkyl, substituted C_1 to C_3 alkyl, aryl, substituted aryl, C_1 to C_3 alkoxy, substituted C_1 to C_3 alkoxy, C_1 to C_3 aminoalkyl, or substituted C_1 to C_3 aminoalkyl; R^4 is H, halogen, CN, NO_2, C_1 to C_6 alkyl, substituted C_1 to C_6 alkyl alkynyl, or substituted alkynyl, C_1 to C_6 alkoxy, substituted C_1 to C_6 alkoxy, amino, C_1 to C_6 aminoalkyl, or substituted C_1 to C_6 aminoalkyl; and R^5 is selected from a trisubstituted benzene ring of a five or six membered ring with 1, 2, or 3 heteroatoms from the group including O, S, SO, SO_2 or NR^6 and containing one or two independent substituents from the group including H, halogen, CN, NO_2, amino, and C_1 to C_3 alkyl, C_1 to C_3 alkoxy, C_1 to C_3 aminoalkyl, COR^F, or NR^{GCORF}; or pharmaceutically acceptable salt thereof. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or inmization of side effects or cyclic menstrual bleeding. Additional uses of the invention include stimulation of food intake.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **179897-89-3**, Benzonitrile, 5-bromo-2-fluoro-
(prepn. of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)
RN 179897-89-3 USPATFULL
CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)

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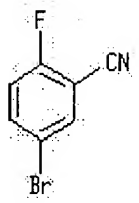


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CA SUBSCRIBER PRICE                                     0.00      -14.70

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STRUCTURE FILE UPDATES:   29 SEP 2004  HIGHEST RN 754169-63-6
DICTIONARY FILE UPDATES:  29 SEP 2004  HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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  conducting SmartSELECT searches.

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L29     STRUCTURE UPLOADED

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L29 HAS NO ANSWERS
L29             STR
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